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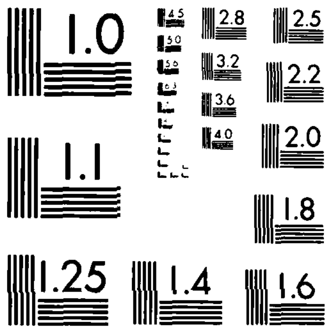

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AFWAL-TR-85-4002

PROCESS MODELS FOR 3D COMPOSITES

Som R. Soni
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Dayton, OHIO 45469

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Mechanics and Surface Interaction Branch
Nonmetallic Materials Division

March 1985

INTERIM REPORT FOR PERIOD SEPTEMBER 1981 - DECEMBER 1983

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85

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AIR FORCE WRIGHT AERONAUTICAL LABORATORIES
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WRIGHT PATTERSON AIR FORCE BASE, OHIO 45433

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This technical report has been reviewed and is approved for publication.

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Carbon-carbon, porous media, process environment, thermo-chemistry, finite element method, fourier transform, flow of fluids.

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This work deals with the process environment modeling of carbon-carbon composites. Capabilities of the process environment model (PEM) computer code developed by Science Applications Incorporated, California, have been discussed. Users instructions for PEM code have been given. Illustrative examples for different phases of processing of carbon-carbon composites are presented. Close form analytical solutions for impregnation analysis have been derived. A comparison between close form solution results and PEM results has been given.

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FOREWORD

This report was prepared by the University of Dayton Research Institute under Air Force Contract No. F33615-81-C-5056, Project No. 241903, Task No. 24190323. The work was administered under the direction of the Nonmetallic Materials Division, Air Force Wright Aeronautical Laboratories, Materials Laboratory, Air Force Systems Command, with Dr. J. M. Whitney (AFWAL/MLBM) as contract monitor.

This report was submitted in December 1983 and covers work conducted from Sept. 1, 1981 to Dec. 1, 1983.

Personnel who contributed to this research are: Som R. Soni and N. J. Pagano.

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SECTION 1
INTRODUCTION

In the subject area of analytical process modeling for improved composites (APIC), extensive work has been reported in [1-4]. The objective of the APIC program was to develop analytical capabilities establishing relationships among the process parameters, composite properties and material response. This capability can provide the means for avoidance of fabrication failures, processing the material with improved, more uniform and repeatable composite properties, and help in further understanding and modifying the process sequence/cycle. The investigation of the influence of process variables on composite microstructure may lead to rapid and low-cost processes which produce carbon-carbon materials with controlled microstructure and desirable properties. To achieve these objectives, two models, namely the process environment model (PEM) and the mechanical model (MIPAC) have been developed at the Science Application Inc., (SAI), Irvine, CA [1]. The PEM deals with the establishment of a relationship between the physical and chemical material properties of constituent materials and processing variables (temperature, temperature rate and pressure), while MIPAC deals with the prediction of the effective thermoelastic properties and strength characteristics of the final state composite material. Computer codes have been developed by SAI for both PEM and MIPAC models for the in-process description of 3-D orthogonal reinforced composites. For this report we have utilized the computer code version available in October 1983.

The primary purpose of the PEM is to predict the pressure and temperature environment for the mechanical model, as shown in Figures 1a-b. In order to carry out such an analysis, it is necessary to account for the process thermochemistry, heat transfer, and flow field for the liquid and gas in all regions of the process can. Given the thermomechanical environment, the mechanical model then predicts the stresses, strains, and displacements in the material, followed by a failure analysis to determine the nature

II. MESH GENERATION

A. Mesh Control Card   Format (6I5)

Columns	Parameter	Description
1-5	MAXI	maximum value of I in mesh* MAXI $\leq$ 25
6-10	MAXJ	maximum value of J in mesh* MAXJ $\leq$ 100
11-15		number of line segment cards
16-20		ignored
21-25		number of material block cards
26-30		maximum relaxation iterations, if blank default of 100 used

*array dimensions for mesh data

B. Line Segment Cards   Format (2(2I3, 2F8.3), 22X, I5)

Columns	Description	
1-3	I	coordinate of first point
4-6	J	coordinate of first point
7-14	R	(X)** coordinate of first point
15-22	Z	coordinate of first point
23-25	I	coordinate of second point
26-28	J	coordinate of second point
29-36	R	(X)+ coordinate of second point
37-44	Z	coordinate of second point
67-71	line segment type (0, 1 or 2)	
	0	point (first point only)
	1	connecting straight line (vertical or horizontal)
	2	connecting straight line ($\pm 45°$ to horizontal)

** in Cartesian coordinates

D. Time Step and Output Options Format (4F10.0, 4I5)

Columns	Parameter		Description
1-10	TSTART		start time — minutes for impregnation & hours for carb. and graph.
11-21	TSTOP		stop time — minutes for impregnation & hours for carb. and graph.
21-30	DT0		time step interval
31-40	TPRINT		minimum print interval selected by time
41-45	NPRINT		minimum print interval selected by number of time steps
46-50	NMAXDT		maximum time steps
51-55	NSK		maximum core storage (zero yields default of 9700)
56-60	NTTDOT	0	no nodal output
		1	print nodal variables only
		2	print nodal variables and time derivatives

E. Equation Solution Sequence Options Format (4I5)

Columns	Description
1-5	number of equations to be solved; if blank, sequence 1, 2 and 3
6-10	code for first equation
11-15	code for second equation
16-20	code for third equation

codes:
1 temperature
2 pressure
3 gas volume fraction

1. ANALYSIS CONTROL

A. Number of cases to be analyzed — Format (I5)

B. Problem Title — Format (8A10)

C. Analysis Options — Format (9I5)

Columns	Parameter		Description
1-5	NPP	0	axisymmetric
		1	plane
6-10	ISTART	0	start at beginning
		1	mesh start file*
		2	continuation run**
	*MCC, LS and MBA cards omitted **initial value card also omitted		
11-15	ISTOP	0	run complete job
		1	generate mesh only
16-20	IOPTN	1	carbonization
		2	impregnation
		3	graphitization
21-25	IPROP	0	material properties are not temperature dependent
		1	material properties are temperature dependent
26-30	IQUAD	0	material properties constant over each triangle
		1	material properties constant over each quadrilateral
31-35	NBF		number of boundary function cards
36-40	NTT		number of time tables
41-45	NUMMAT		number of materials (impregnant and preform)

APPENDIX A

PEM COMPUTER CODE USER INSTRUCTIONS

REFERENCES

1. W.C. Loomis, F.K. Tso, R.B. Dirling Jr. and C. N. Heightland, Science Applications Inc., California, Personal Communication.

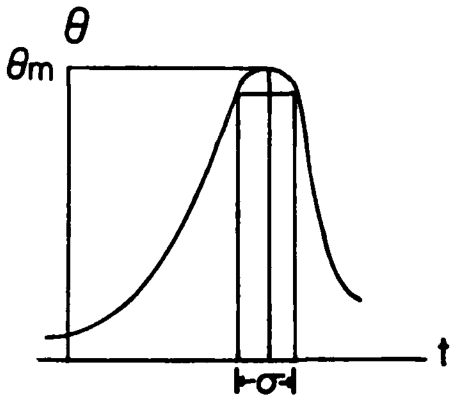
2. W.C. Loomis, F.K. Tso, C.N. Heightland and J.J. Glatz, Science Applications Inc., California, Personal Communication.

3. W.C. Loomis, F.K. Tso, R.B. Dirling Jr. and C.N. Heightland, Science Applications Inc., California, Personal Communication.

4. W.C. Loomis, F.K. Tso and C.N. Heightland, Science Applications Inc., Personal Communication.

5. C.N. Heightland, Science Applications Inc., California, Personal Communication.

6. R.E. Collins, "Flow of Fluids Through Porous Media," Reinhold Publishing Corporation, New York, 1961.



Reaction midpoint temperature and its time width.

where

H_r = heat of reaction

$\dot{m}_g$ = rate of reaction/unit initial mass.

$\Delta\tilde{w}$ = total weight loss/unit initial mass.

Θ_m = reaction midpoint temperature

σ = width of reaction time

s = gas volume fraction

ϕ = porosity

ρ_ℓ = liquid density

$$f(u) = \frac{1}{\sqrt{2\pi}} e^{-u^2/2}$$

7. Thermophysical properties of each material:

   (a) Material Porosity (ϕ).
   (b) Change of pitch density with pressure ($\frac{\partial\rho_\ell}{\partial P}$).
   (c) Material property table for each temperature for the following properties:
      (i) Thermal conductivity (K)
      (ii) Gas molecular weight (M_q)
      (iii) Density of solid, liquid and gas ($\rho_s, \rho_\ell, \rho_g$)
      (iv) Viscosity of liquid and gas (M_ℓ, M_g)
      (v) Specific heats of solid, liquid and gas ($C_{ps}, C_{p\ell}, C_{pg}$)
      (vi) Permeability (K^P)
      (vii) Material emissivity.

4. Capillary action equation constants

a_i (i=1,...,4) and $\bar{c}$ for

$$p_c = \bar{c} \left\{ a_1 s + a_2 \left[\frac{1}{(a_3 - s)^2} - a_4 \right] \right\}$$

$$s = 1 - s_w$$

s_w = wetting fluid saturation

(saturation of the void volume with wetting fluid)

5. Various constants required:

(a) Universal gas constant, R (perfect gas law).

(b) Stefan-Boltzman constant (for graph. only).

(c) Gravitational constant, g.

(d) Energy conversion constant, J_c.

(e) Carbonization rate, T_c.

6. Reaction details for the chemical dissipation function ϕ_c.

$$\phi_c = - \sum_{i=1}^{3} H_{ri} \, \dot{\tilde{m}}_{gi} (1-s) \phi \rho_p \qquad \text{(for carbonization only)}$$

$$i = \begin{cases} 1, & \text{pitch decomposition} \\ 2, & \text{mesophase formation} \\ 3, & \text{carbon formation} \end{cases}$$

$$\dot{\tilde{m}}_{gi} = \frac{\Delta W_i}{\sigma_i} f\left(\frac{\theta - \theta m_i}{\sigma_i}\right)$$

SECTION II

MATERIAL CONSTITUENT PROPERTIES, ASSUMPTIONS AND OTHER REQUIREMENTS FOR PEM

A. FIELD THEORIES

For the development of the computer code the following field theories are used:

a) Fourier's law of heat conduction.

b) Darcy's law of flow of fluids through porous media.

For further details the reader is advised to consult reference [1].

B. INPUT DATA REQUIREMENTS FOR IMPREGNATION ANALYSIS

1. Billet (preform) Dimensions
2. The following material properties

   (a) Change of pitch density with pressure

$$\frac{\partial \rho}{\partial P}, \quad (C = \frac{1}{\rho}\frac{\partial \rho}{\partial P})$$

   (b) Solid material porosity (ϕ)

$$\phi = 1 - \frac{V_{solid}}{V_{bulk}}$$

   (c) Liquid pitch density (ρ)

   (d) Liquid Pitch viscosity (μ)

   (e) Anisotropic permeability of the material (K^P)

   (f) Boundary conditions

C. INPUT DATA REQUIREMENTS FOR CARBONIZATION AND GRAPHITIZATION ANALYSES

1. Boundaries of billet dimensions, liquid & preform constituents.
2. Process cycle: Distribution of temperature & pressure with time.
3. Initial and boundary conditions for temperature, pressure and gas volume fraction.

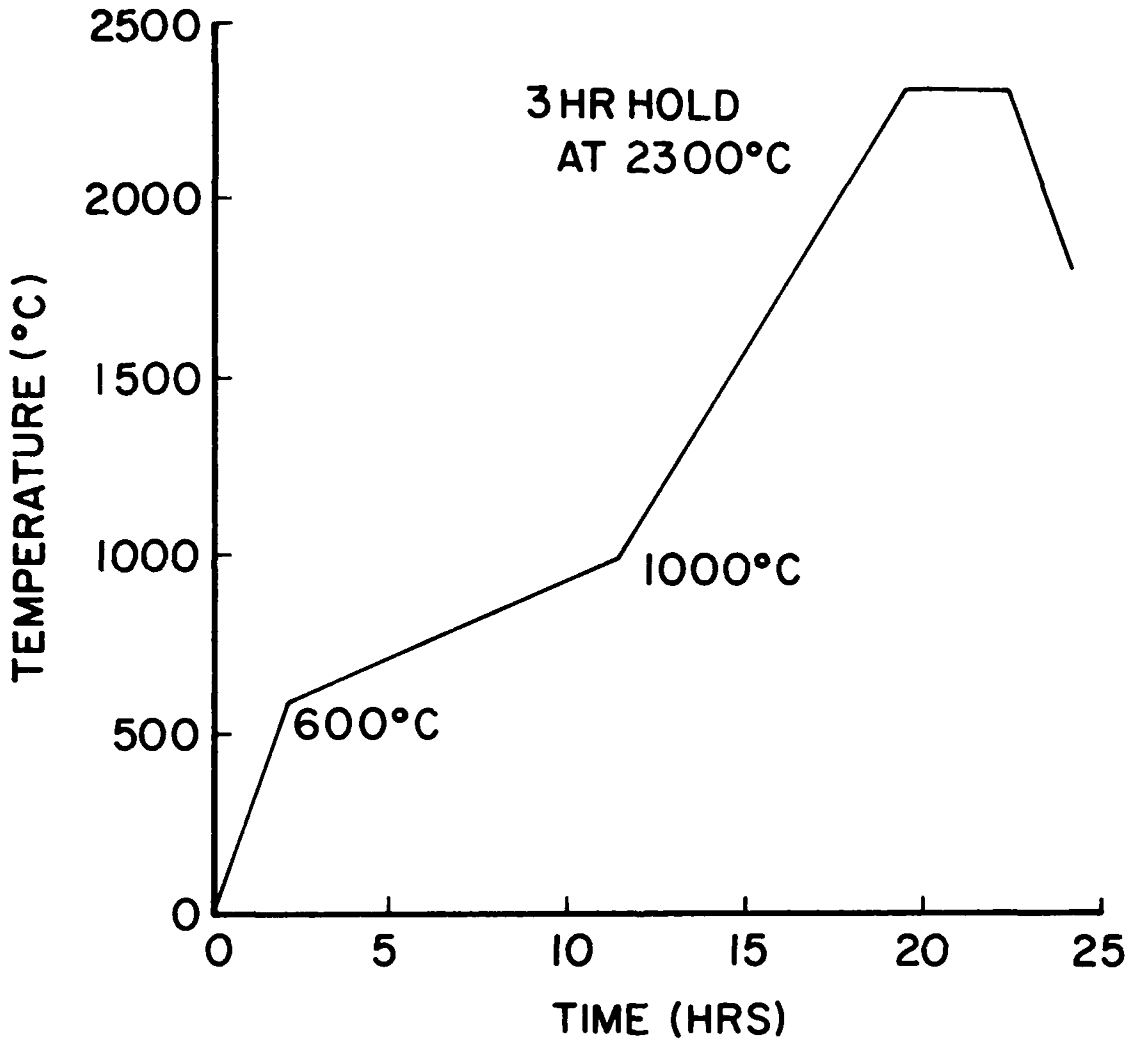


Figure 2b. Graphitization Schedule for APIC Idealized Composite.

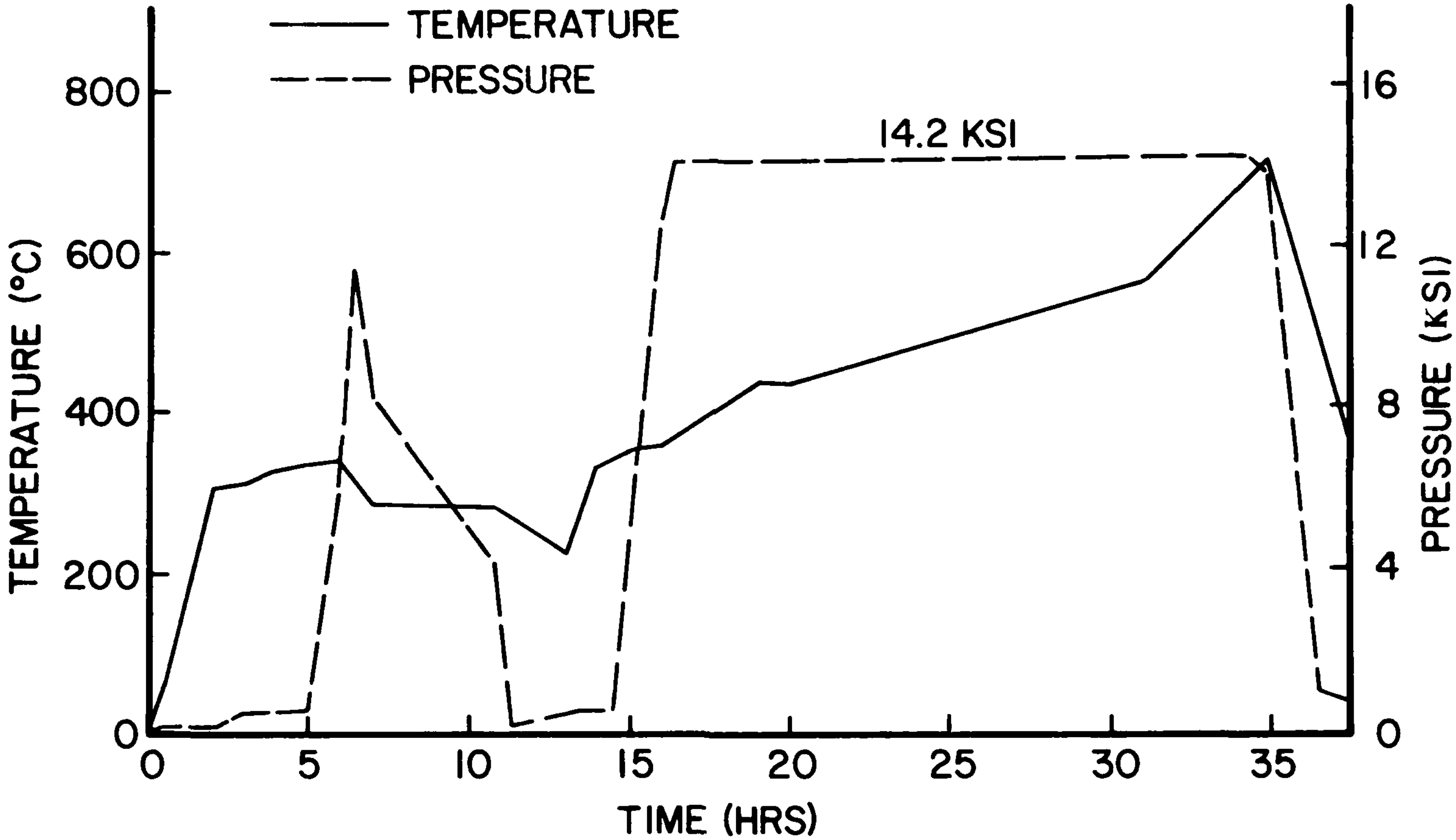


Figure 2a. APIC Carbonization Cycle.

Processing Sequence

1. Weave preform: Carbon fibers are stiffened and woven in a 3-D configuration.
2. Cage preform: The preform is placed in a cage to allow adequate access of the impregnant and constrained gently to avoid distortion.
3. Preform is loaded into the processing can and fillers are added.
4. Impregnation: Can is heated to a prescribed temperature in the impregnation unit and the impregnant is allowed to flow into the preform at temperature and pressure conditions.
5. Carbonization: The can with impregnated billet is sealed/vented and subjected to a prescribed process cycle. A carbonization process cycle used by SAI [1] is given in Figure 2a.
6. Graphitization: The carbonized billet is then subjected to a graphitization process cycle. A typical graphitization process cycle is given in Figure 2b.
7. Last three steps (step 4 through step 6) are repeated until desired properties are achieved.

and extent of any damage which might occur. This must be repeated for incrementally applied loading until the entire process is modeled. In principle, it is also possible that the output of the mechanical model can alter the true response of the process environment model by changing material thermal conductivities and permeabilities at local damage sites. This is shown by the feedback path indicated in the Figure 1b, and while possible, it is not a real time link between computer codes. Approximate satisfaction of this link can be provided, however, through repetition of analysis and the use of engineering judgement.

In this report we will concentrate on the process environment model. All the required (input) material properties in three different phases of processing i.e. impregnation, carbonization and graphitization are listed in the following section. User's instructions for the PEM computer code are given in Appendix A. These instructions are for the analysis of impregnation, carbonization and graphitization as well as the graphics post processor. The user's instructions for computer codes for 3D thermal and diffusion property predictions and the degree of graphitization analysis are not given in this report. A number of illustrative examples are treated and input/output for these problems are explained. The temperature dependent material properties used in these problems are exhibited in figures. The results for the sample problems are presented in graphical form. Independently, we have derived closed form solutions for impregnation of the billet in Cartesian and cylindrical polar coordinates for certain special cases. A comparison between the PEM results and closed form solution results has been made. There exists a good agreement between the converged results obtained by the PEM and closed form solution for both the rectangular and cylindrical polar coordinate systems.

For the complete processing of 3-D carbon-carbon material the following processing sequence may be employed:

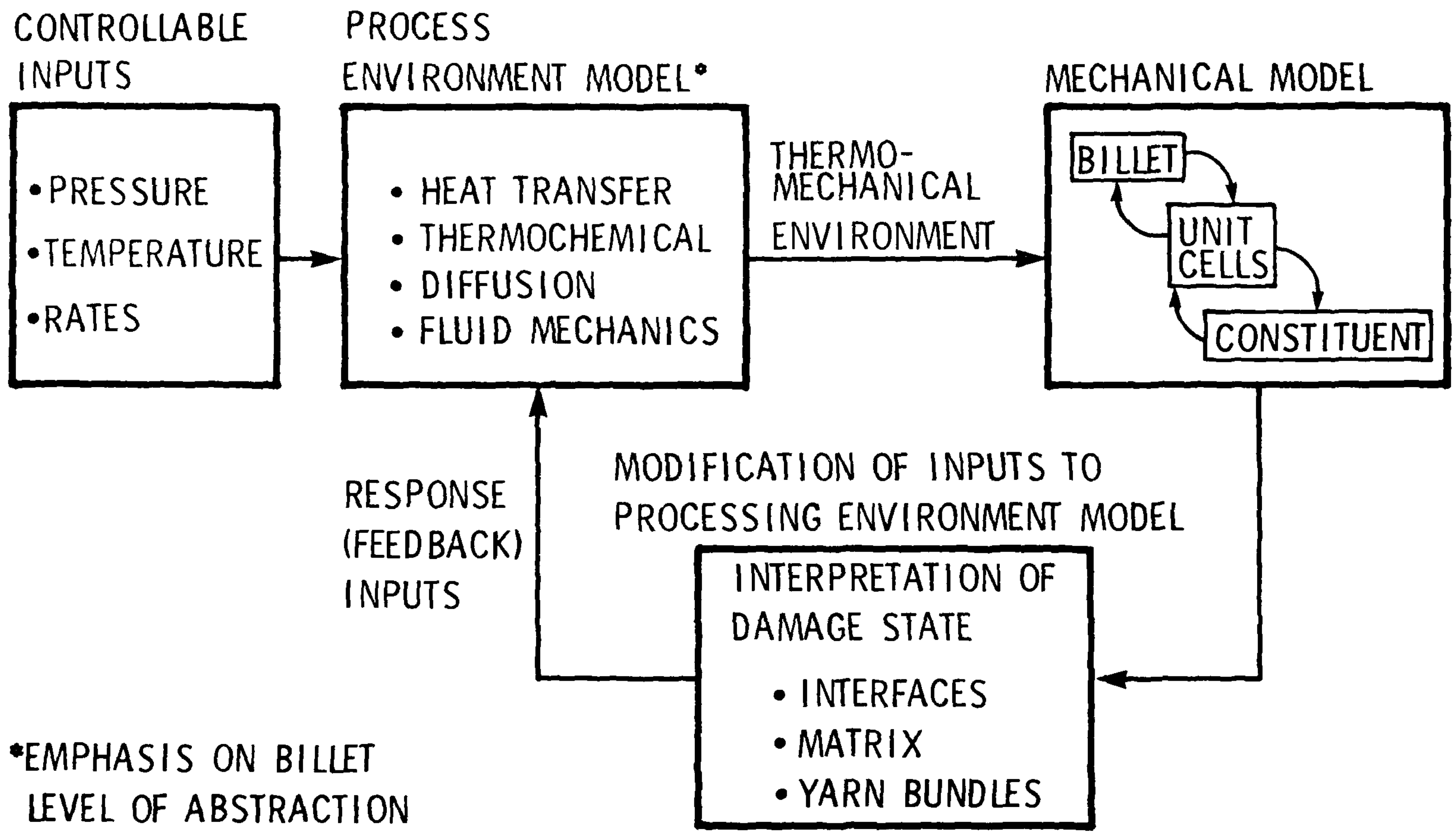
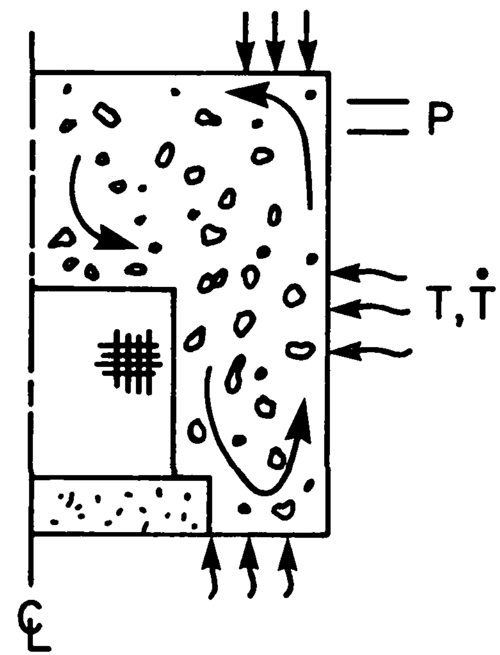


Figure 1b. Relationship Between Process Environment Model and Mechanical Model.

FINITE ELEMENT TRANSIENT FIELD SOLUTIONS



IMPREGNATION
CARBONIZATION
GRAPHITIZATION

3D THERMAL AND DIFFUSION PROPERTY PREDICTION

DEGREE OF GRAPHITIZATION ANALYSIS

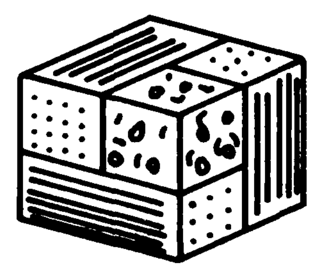
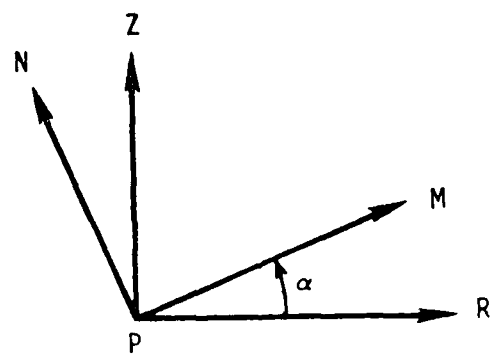


Figure 1a. Major Components of Process Environment Model.

C. Material Block Assignment Cards Format (5I5, F10.0)
(material outside billet must be material number one)

Columns	Description
1-5	material definition number (1-12)
6-10	minimum I boundary
11-15	maximum I boundary
16-20	minimum J boundary
21-µ5	maximum J boundary
26-35	material property inclination angle in degrees (usually blank)

Note: the orientation of the M-N-P material coordinate system with respect to the R-Z-P body coordinate system is shown below. The angle is input via a MATERIAL BLOCK ASSIGNMENT CARD. Both are right handed systems.



III. BOUNDARY FUNCTIONS Format (6I5, 2F10.0)

Each card defines input data for a group of nodal points bounded by I1, I2, J1, J2, on the external boundary of the body. For a line, I1 = I2 or J1 = J2. For a point, I1 = I2 and J1 = J2. The time variation for each card input below is specified by TIME TABLE CARDS.

Columns	Description
1-5	KIND, the type of boundary function (1 - temp., 2 - pressure, 3 - gas volume fraction 4 - graphitization source temp.)
6-10	I1, the initial value of I
11-15	J1, the initial value of J
16-20	I2, the final value of I
21-25	J2, the final value of J
26-30	NTABLV, corresponding time table identification number (zero if function does not vary with time)
31-40	V1, the value of the function at (I1, J1)
41-50	V2, the value of the function at (I2, J2)

IV. INITIAL VALUES Format (30X, 3F10.0)

The initial value of temperature, pressure, and/or gas volume fraction for each equation to be solved, input in problem sequence order.

Columns	Description
31-40	constant initial value, first equation
41-50	constant initial value, second equation
51-60	constant initial value, third equation

V. AUXILIARY EQUATION CONSTANTS

A. Capillary Action Equation Format (5F10.0)

Columns	Description
1-10	capillary pressure constant, a_1
11-20	capillary pressure constant, a_2
21-30	capillary pressure constant, a_3
31-40	capillary pressure constant, a_4
41-50	capillary pressure strength, $\bar{c}$

$$p_c = \bar{c} \left\{ a_1 s + a_2 \left[\left(\frac{1}{a_3 - s} \right)^2 - a_4 \right] \right\}$$

(a_1 to a_4 are dimensionless and $\bar{c}$ is in PSI)

B. Material Constants Format (7F10.0)

Columns	Description
1-10	universal gas constant, $\bar{R}$ -(BTU/lb. mole-°R)
11-20	residual liquid, $S_{\ell r}$ (normally blank)
21-30	residual gas, S_{gr} (normally blank)
31-40	Stefan-Boltzman constant -(BTU/Hr in^2 °R^4) (graphitization problems only)
41-50	gravitional acceleration, g -(in/Hr^2)
51-60	gravitional constant, g_c - (in/lb-F Hr^2)
61-70	energy conversion constant, J_c(in lb-f/BTU)
71-80	carbonization rate, T_c

C. Decomposition Reaction Format (4F10.0)

Columns	Description
1-10	total gas evolved, Q_{o1}
11-20	reaction midpoint temperature, T_{M1}
21-30	reaction temperature range, σ_1
31-40	heat of reaction, H_{r1}

D. Mesophase Reaction Format (4F10.0)

Columns	Description
1-10	total gas evolved, Q_{o2}
11-20	reaction midpoint temperature, T_{M2}
21-30	reaction temperature range, σ_2
31-40	heat of reaction, H_{r2}

E. Graphitization Reaction Format (4F10.0)

Columns	Description
1-10	total gas evolved, Q_{o3}
11-20	reaction midpoint temperature, T_{M3}
21-30	reaction temperature range, σ_3
31-40	heat of reaction, H_{r3}

VI. MATERIAL THERMOPHYSICAL PROPERTIES
(one set of input properties per material)

A. Material Identification Format (4I5, 3F10.0)

Columns	Description
1-5	identification number (1-12)
6-10	number of temperatures (1-12)
11-15	isotropy parameter 0 anisotropic material 1 isotropic material
16-20	material type 1 solid 2 liquid 3 porous (normally used)
21-30	change of pitch density with pressure
31-40	material porosity
41-50	solid material density

B. Material Property Table* Format (7F10.0/10X, 5F10.0/10X, 6F10.0)

Columns	Description
First Card	
1-10	temperature, T
11-20	conductivity, K_{MM} — See Material Block Assignment Cards, II C.
21-30	conductivity, K_{NN} — See Material Block Assignment Cards, II C.
31-40	gas molecular weight, M_g
41-50	Blank
51-60	liquid pitch density, ρ_ℓ
61-70	change of pitch density with temperature
Second Card	
11-20	gas viscosity, μ_g
21-30	liquid pitch viscosity, μ_ℓ
31-40	yarn or filler specific heat, C_{ps}
41-50	permeability, K_r^p or K_x^p
51-60	permeability, K_z^p
Third Card	
11-20	gas density, ρ_g
21-30	gas specific heat, C_{pg}
31-40	liquid pitch specific heat, $C_{p\ell}$
41-50	material emissivity,

*Units for these quantities are mentioned in Figures 8-19 also see Tables 3 and 4.

VII. TIME TABLE INFORMATION

A. Time Table Identification — Format (2I5)

Columns	Description
1-5	identification number
6-10	number of ordered pairs ($\leq$ 20)

B. Time Tables — Format (8F10.0)

Columns	Description
1-10	first table time
11-20	first function value
21-30	second table time
31-40	second function value
.	
.	
.	

VIII. TERMINATION OF INPUT

A. End of Case Card — Format (2A10)

enter, "END OF CASE"

B. End of Data Card — Format (2A10)

enter,"END OF DATA"

APPENDIX B

POST-PROCESSOR AND GRAPHICS CODE USER INSTRUCTIONS

Post processor and graphics code developed by SAI [1] is helpful in obtaining contour plots of various parameters during processing. This code is written such that a SC-4020 plotter is used - and therefore requires the relevant plot routine library attached. Data preparation instructions are as follows:

1. TITLE AND CONTROL

A. Title Format (8A10)

B. Options Control Format (5I5)

Columns	Description		
1-5	IDEN	0	no density calculation
		1	calculate density
6-10	IMESH	0	no mesh plot
		1	plot mesh
11-15	ICON	0	no contour plot
		1	plot contours
16-20	IPLOT	0	standard plots
		1	non-standard plots (plot scale card required)
21-25	ISTART	0	data on tape 8
		1	data on tapes 21,22,23, and 24

II. MATERIAL PROPERTY Format (2I5/2F10.0)
(omitted if density is not calculated)

A. Material Identification

Columns	Description
	First Card
1-5	number of materials
6-10	number of ordered pairs in pitch density table ($\leq$ 12)
	Remaining Cards - (one card each material)
1-10	porosity
11-20	solid constituent density

B. Pitch Density Table Format (8F10.0)

Columns	Description
1-10	first table temperature
11-20	first table density
21-30	second table temperature
31-40	second table density
.	
.	
.	

III. PLOT SCALE OPTION Format (5F10.0)
(omitted if standard plot selected)

Columns	Description
1-10	minimum R coordinate plotted
11-20	maximum R coordinate plotted
21-30	minimum Z coordinate plotted
31-40	maximum Z coordinate plotted
41-50	rotation parameter (if 1.0, Z-axis is vertical; if 0.0, Z-axis is horizontal)

IV. CONTOUR PLOTTING OPTION
(omitted if contour plots not selected)

A. Plot Control Format (3I5)

Columns	Description
1-5	number of variables to be plotted
6-10	NTIME number of times to be plotted (NTIME $\leq$ 10)
11-15	KIND 0 first NTIME responses plotted 1 response times input

B. Plot Times Format (8F10.0)
(omitted if KIND = 0)

Columns	Description
1-10	first time requested
11-20	second time requested
21-30	third time requested

.
.
.

C. Plot Function Options

One card is required for each variable to be plotted. A card may utilize either of the two options defined below.

i. Automatic Contour Selection Format (8I5, 2A10)

Columns	Description
1-5	plot code 1 temperature
	2 pressure
	3 liquid fraction
6-10	number of contours desired (enter as negative. $\leq$ 10)
11-15	first of three acceptable contour divisions (default = 1)
16-20	second of three acceptable contour divisions (default = 2)
21-25	last of three acceptable contour divisions (default = 5)
26-30	variable range plotted
	0 entire range
	1 non-negative range
	-1 non-positive range
31-35	symbol frequency (default = 4)
36-40	range selection method
	0 based on current time
	1 based on total time
	(Tape 8 must be used, not Tapes 21, 22, 23 and 24 ISTART = 0)
41-50	variable's units, printed on plot
51-60	time units, printed on plot (Hours)

ii. Specified Contour Values Format (2I5,30X,2A10/8F10.0)

Columns	Description		
	First Card		
1-5	plot code	1	temperature
		2	pressure
		3	liquid volume fraction
		4	density
6-10	number of contours ($\leq$ 10)		
41-50	variable's units, printed on plot		
51-60	time units, printed on plot		
	Second Card		
1-10	first contour to be plotted		
11-20	second contour to be plotted		
.			
.			
.			

V. TERMINATION OF INPUT

End of Data Card

Format (2A10) enter "END OF DATA"

APPENDIX C
PEM ILLUSTRATIONS

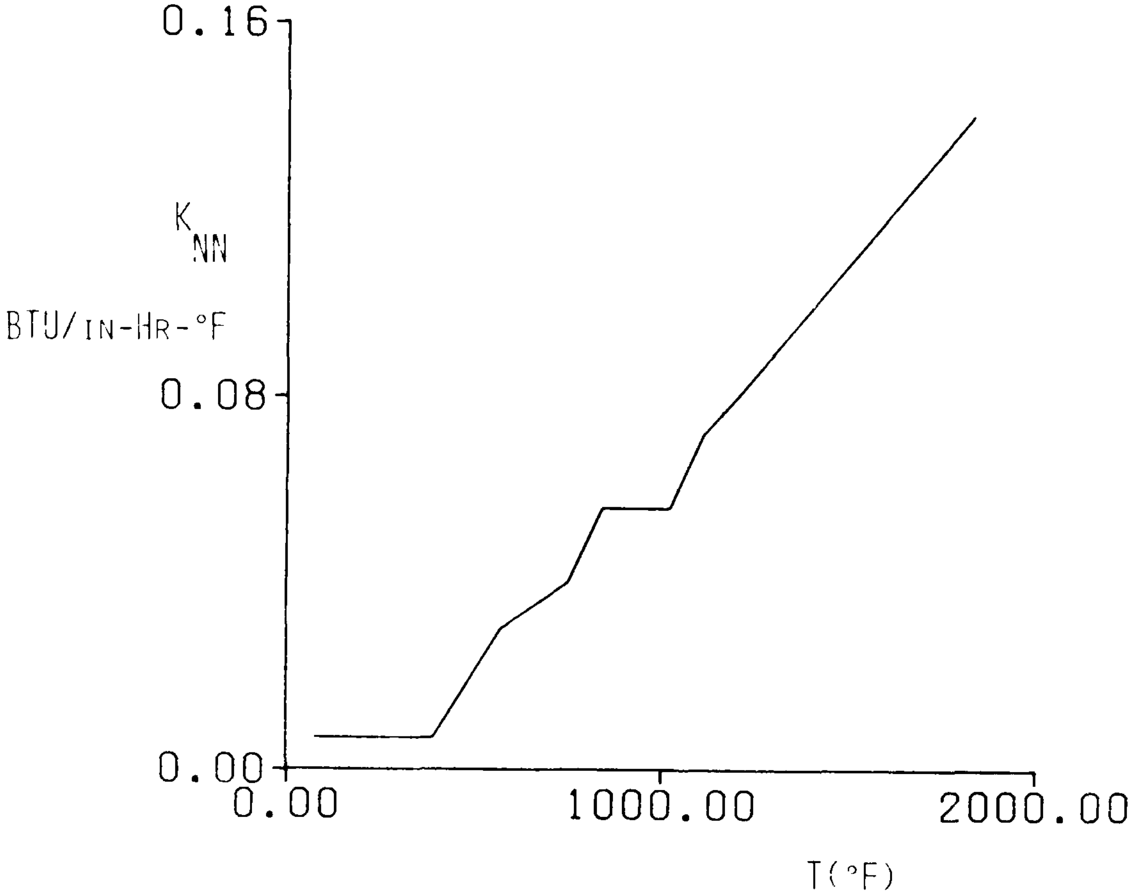


Figure 9. Liquid Thermal Conductivity K_{NN} Versus Temperature T (°F).

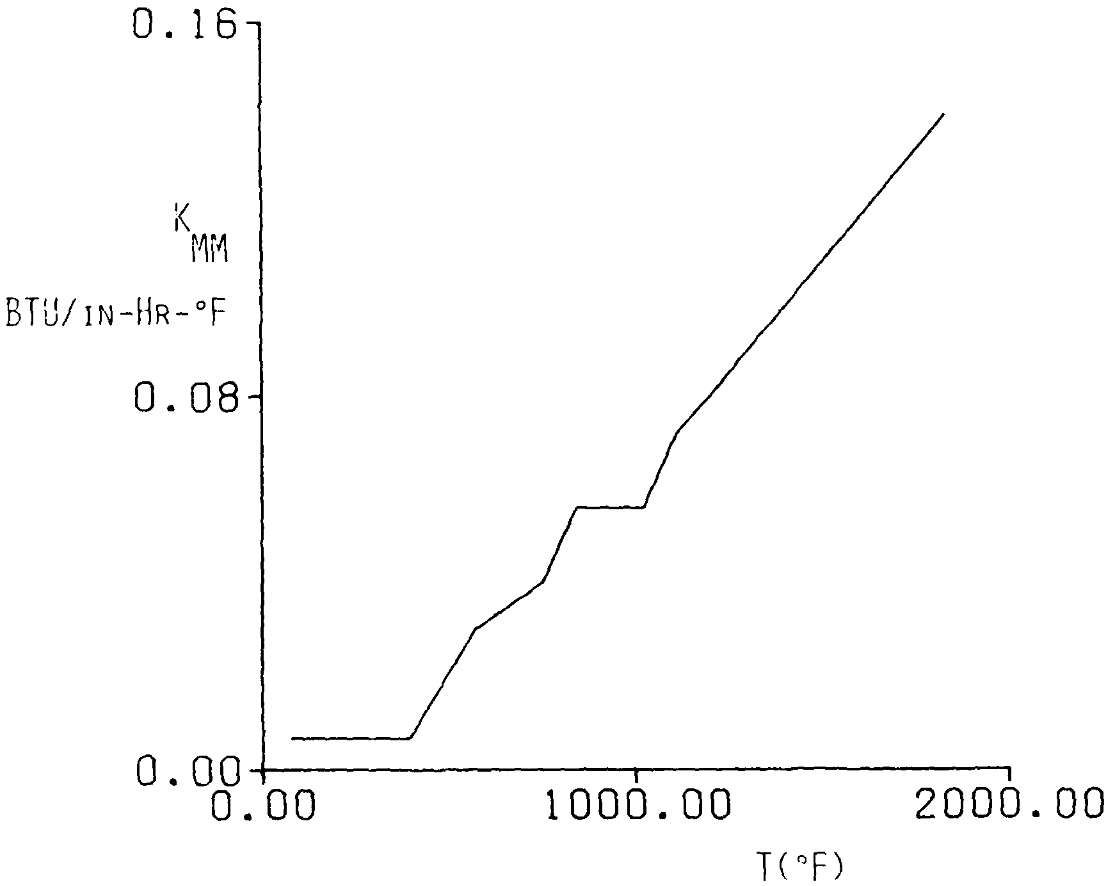


Figure 8. Liquid Thermal Conductivity K_{MM} Versus Temperature T (°F).

TABLE 3

LIQUID MATERIAL PROPERTY TABLE CORRESPONDING
TO THE INPUT DATA INSTRUCTIONS GIVEN ON PAGE 21 i.e.

T, K_{MM}, K_{NN}, M_g, ρ_ℓ, $\frac{\partial \rho_\ell}{\partial T}$ Format (4F10.0, 10X, 2F10.0)

μ_g, μ_ℓ, C_{ps}, K_x^ρ, K_z^ρ Format (10X, 5F10.0)

[illegible]$_g$, C_{pg}, $C_{p\ell}$ Format (10X, 4F10.0)

```
.5370E+03 .6800E-02 .6800E-02 .1500E+030.           .4650E-01-.1004E-04
          .4026E-12 .2013E-04 .2980E+00 .1000E-06 .1000E-06
          .6538E-04 .2000E+00 .3250E+000.
.6720E+03 .6800E-02 .6800E-02 .1500E+030.           .4530E-01-.1004E-04
          .7247E-12 .2013E-04 .3120E+00 .1000E-06 .1000E-06
          .5236E-04 .2150E+00 .3850E+000.
.76[illegible]E+03 .6800E-02 .6800E-02 .1500E+030.           .4470E-01-.5530E-05
          .[illegible]E-12 .2416E-08 .3220E+00 .1000E-06 .1000E-06
          .4[illegible]37E-04 .2240E+00 .1217E+010.
.8520E+03 .6800E-02 .6800E-02 .1500E+030.           .4440E-01-.7190E-06
          .8657E-12 .2536E-08 .3300E+00 .1000E-06 .1000E-06
          .4136E-04 .2330E+00 .4390E+000.
.1032E+04 .3000E-01 .3000E-01 .1500E+030.           .4410E-01 .1970E-04
          .1035E-11 .4429E-07 .3486E+00 .5000E-08 .5000E-08
          .3379E-04 .2489E+00 .3926E+000.
.1212E+04 .4000E-01 .4000E-01 .1360E+020.           .4380E-01 .2360E-04
          .1168E-11 .2013E-04 .3660E+00 .1000E-09 .1000E-09
          .2980E-04 .2620E+00 .5170E+000.
.1302E+04 .5600E-01 .5600E-01 .7500E+010.           .4365E-01 .2530E-04
          .1260E-11 .2013E-04 .3750E+00 .1000E-09 .1000E-09
          .2691E-04 .2650E+00 .5050E+000.
.1392E+04 .5600E-01 .5600E-01 .2280E+020.           .4350E-01 .6630E-06
          .1329E-11 .2013E-04 .3840E+00 .1000E-09 .1000E-09
          .2521E-04 .2680E+00 .4760E+000.
.1482E+04 .5600E-01 .5600E-01 .1070E+030.           .4335E-01-.6590E-05
          .13[illegible]9E-11 .2013E-04 .3920E+00 .1000E-09 .1000E-09
          .2366E-04 .2710E+00 .4300E+000.
.1572E+04 .7200E-01 .7200E-01 .4770E+020.           .4320E-01-.8800E-05
          .1449E-11 .2013E-04 .4000E+00 .1000E-09 .1000E-09
          .2210E-04 .2740E+00 .4300E+000.
.1662E+04 .9000E-01 .9000E-01 .2780E+020.           .4305E-01-.9660E-05
          .1514E-11 .2013E-04 .4077E+00 .1000E-09 .1000E-09
          .2090E-04 .2770E+00 .4077E+000.
.2292E+04 .1400E+00 .1400E+00 .1600E+020.           .6400E-01 .2[illegible]0E-04
          .1684E-11 .2013E-04 .4530E+00 .1000E-09 .1000E-09
          .1538E-04 .3090E+00 .4530E+000.
```

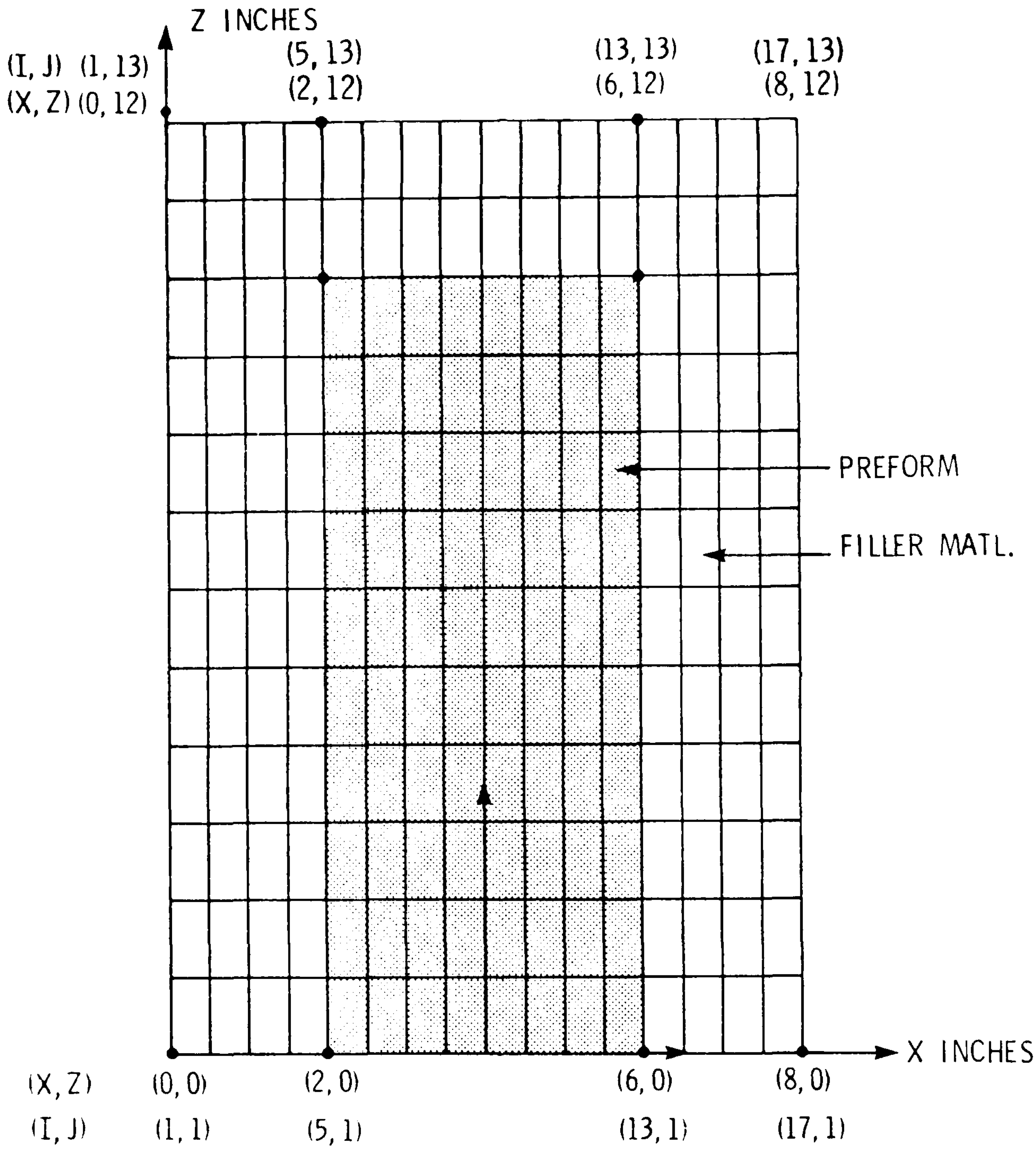


Figure 7. Finite Element Grid for a Billet.

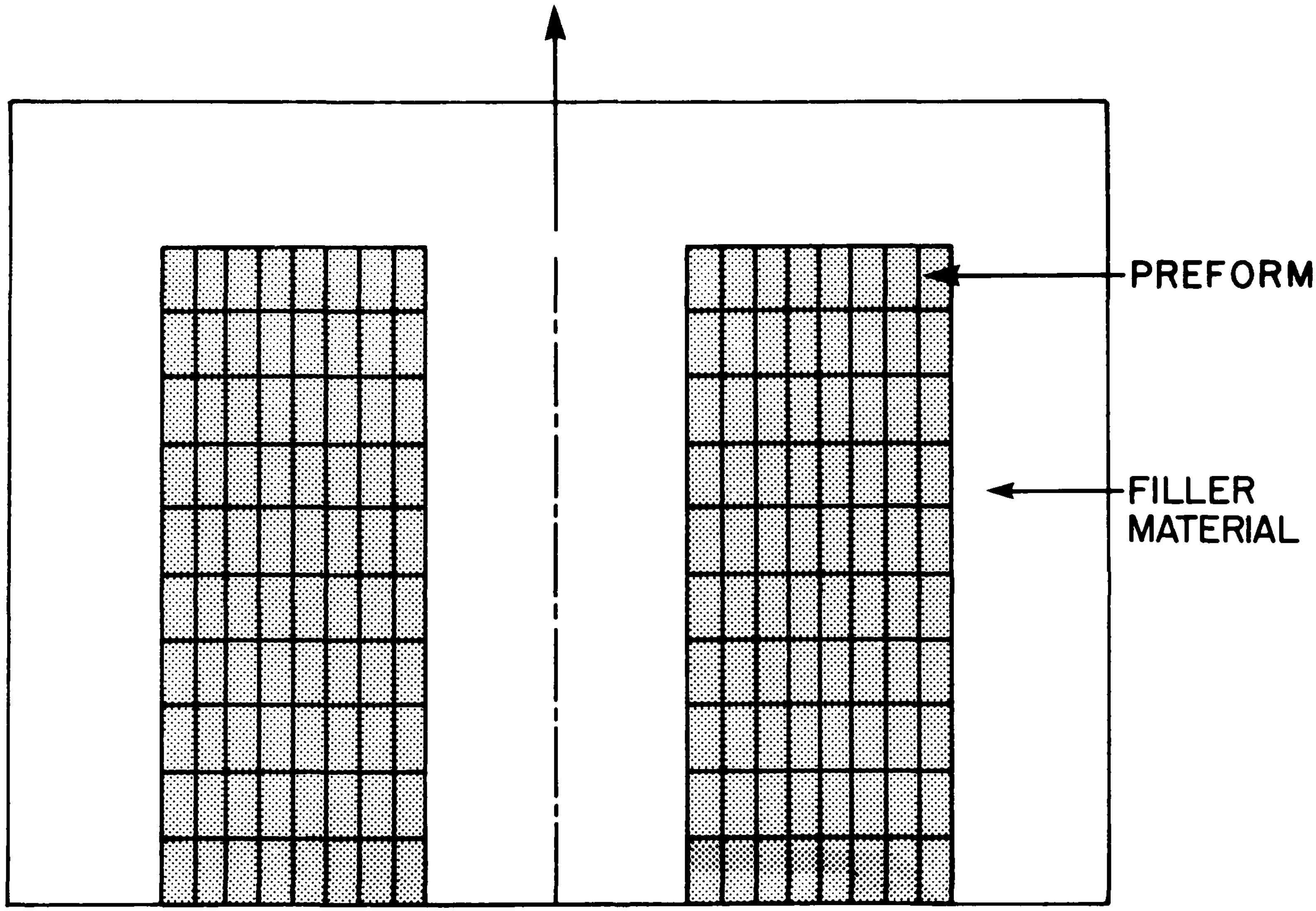


Figure 6. Two Billet Can for Carbonization.

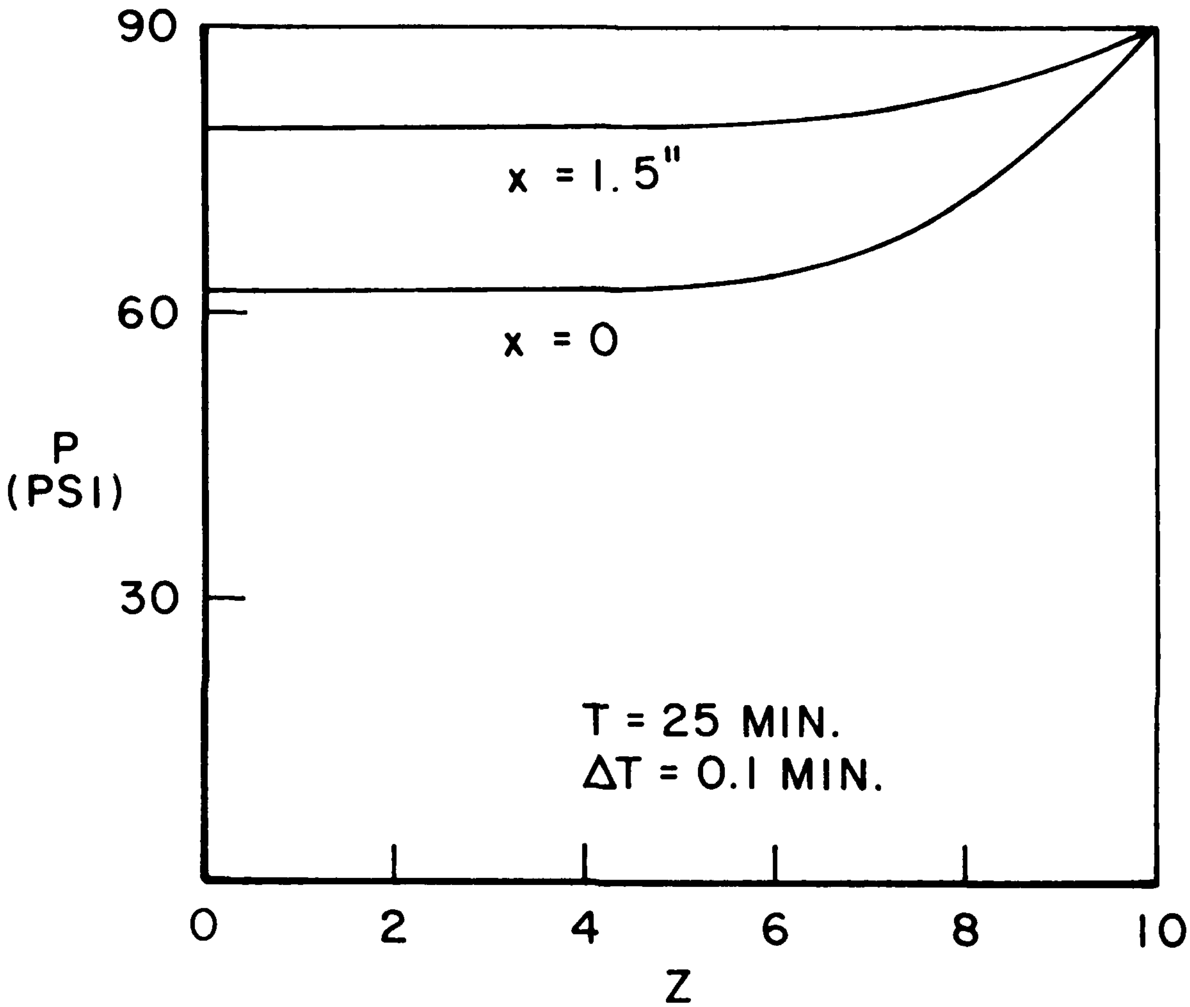


Figure 5. Pressure Distribution in the Billet at Different Points after Twenty Five Minutes of Impregnation, PEM Code Calculations.

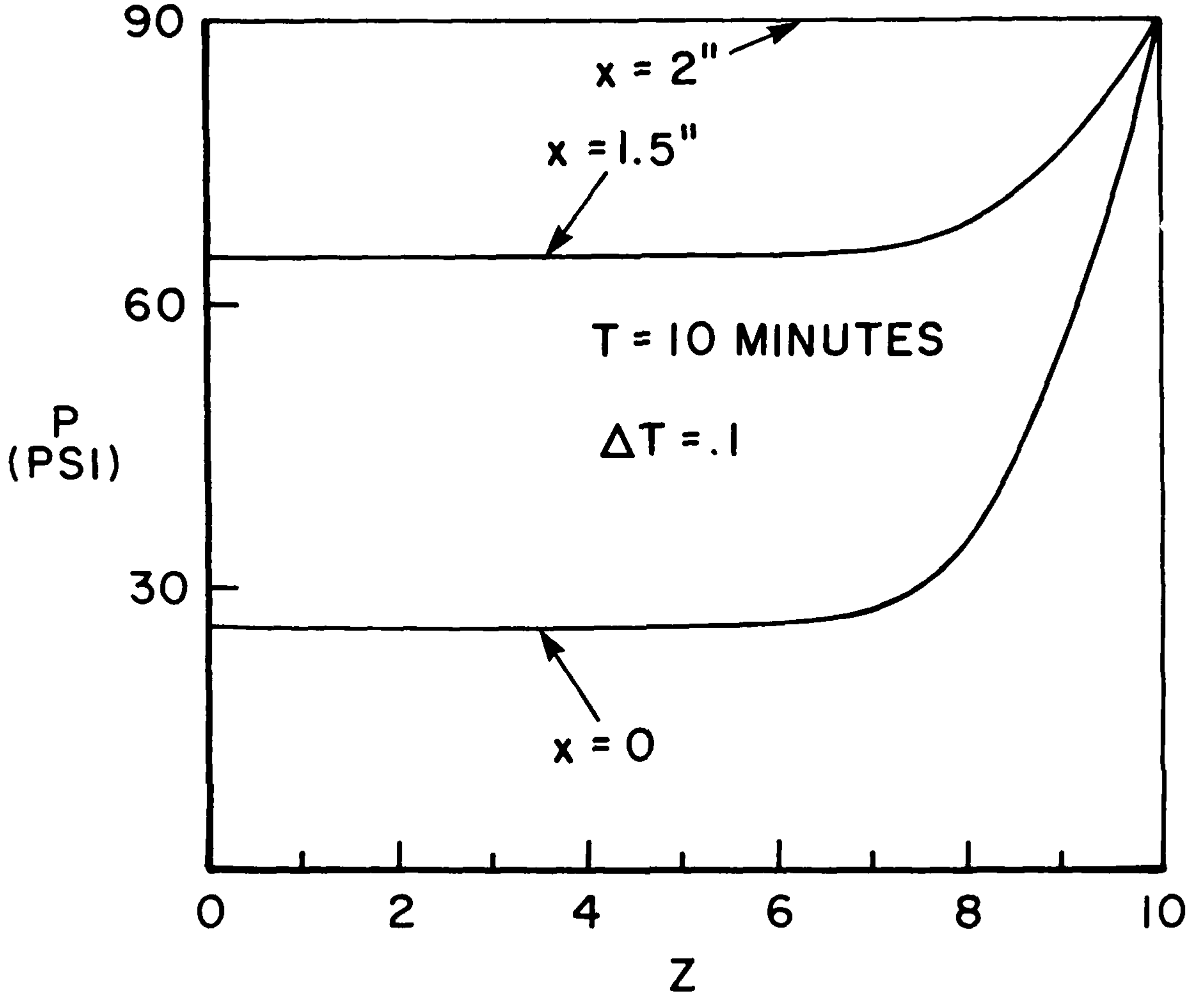


Figure 4. Pressure Distribution in the Billet at Different Points after Ten Minutes of Impregnation, PEM Code Calculation.

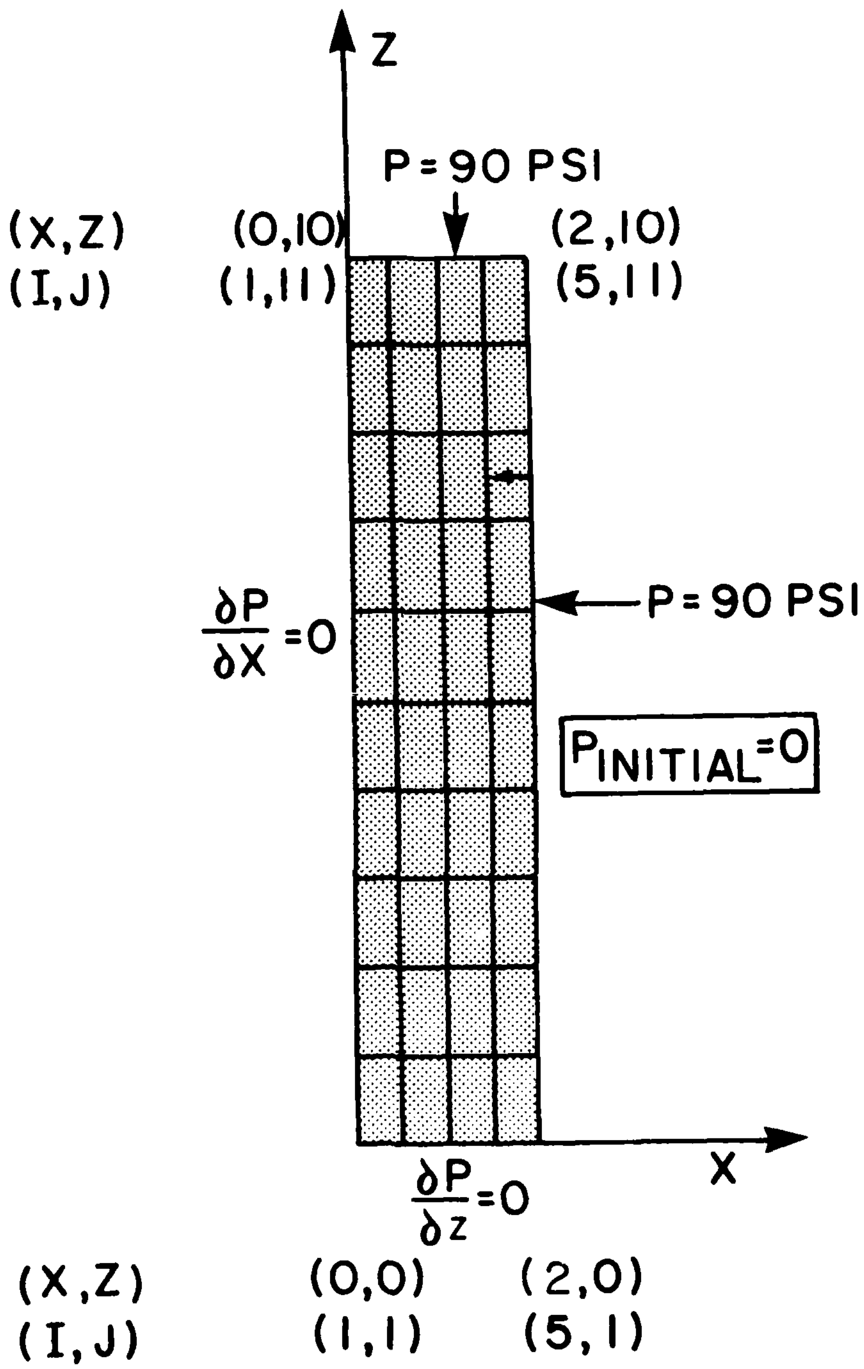


Figure 3. Billet Preform Finite Element Model.

TABLE 2

INPUT DATA FOR IMPREGNATION ANALYSIS
OF THE BILLET GIVEN IN FIGURE 3

```
                 I M A G E S   O F   D A T A   C A R D S   F O R   N C A S E  = 1

      ---------------------------------------------------------------------------------
      1        10        20        30        40        50        60        70        80
      ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?
      ---------------------------------------------------------------------------------
  1-   A"*IC" BILLET                                                                   -
  2-     1    0    0    2    0    0    2    0    1                                    -
  3-0.        40.       0.1       400.           1 400     0    1                     -
  4-     1    2                                                                        -
  5-     5   11   10        1 150                                                      -
  6-  1  1  0.        0.    5  1 2.     0.                                     1       -
  7-  5  1 2.     0.        5 11 2.     10.                                    1       -
  8-  5 11 2.     10.       1 11 0.     10.                                    1       -
  9-  1  1 0.     0.        1 11 0.     10.                                    1       -
 10- -1                                                                                -
 11-     1    1    5    1   11                                                         -
 12-     2    5    1    5   11     0 90.0     90.0                                     -
 13-     [illegible]    1   11    5   11     0 90.0     90.0                           -
 14-                                                                                   -
 15-                                                                                   -
 16-                                                                                   -
 17-                                                                                   -
 18-                                                                                   -
 19-                                                                                   -
 20-     1    1    1    3 5.2731E-7 0.31                                               -
 21-                                                  0.045586                         -
 22-                    2.4155E-7          7.5000E-147.5000E-14                        -
 23-END OF CASE                                                                        -
      :----:----:----:----:----:----:----:----:----:----:----:----:----:----:----:----:
```

and permeability (Table 5). The contour plots of all the significant parameters at different times during processing for the three cases are given in Figures 26-58. For each case, temperature contours are given at six values of time, starting from T = 5 hours to T = 30 hours, with a gap of five hours. Pressure and density contours are plotted at two times, T = 5 hours and T = 30 hours. Also, the temporal variation in temperature, pressure, density and gas volume fraction at point (4",6") has been shown for each case (Figures 36, 47, 58). Those are not a part of the FEM code. The carbonization and graphitization problems solved here are independent of each other.

$$P\,(2'',z,t) = 90 \text{ PSI} \quad 0 \le z \le 10''$$

$$P\,(x,10'',t) = 90 \text{ PSI} \quad 0 \le x \le 2''$$

$$\left.\frac{\partial p}{\partial x}\right|_{x=0} = 0$$

$$\left.\frac{\partial p}{\partial z}\right|_{z=0} = 0$$

$$P(x,z,0) = 0$$

The input data for this analysis is given in Table 2. The pressure distributions as a function of spacial coordinates and time are given in Figures 4 and 5.

For carbonization analysis two impregnated billets, as shown in Figure 6, XZ-plane, are considered to be placed in a processing can. Because of geometric symmetry, half of the can was modeled. The boundary conditions imposed in this problem are also shown in Figure 6. The finite element model shown in Figure 7 has been used. The temperature dependent material properties of the billet preform and liquid pitch are given in Tables 3, 4 and 5. The properties given in Tables 3 and 4 are given in graphical form in Figures 8-23. The carbonization process temperature schedule is given in Figure 24. The carbonization analysis is done up to 30 hours of processing, Table 1. Because of the length of the processing time and the size of the problem, the analysis was conducted in two runs for each set of preform porosity and density values, i.e. (1) $0 \le T \le 15$ (hrs), (2) $15 \le T \le 30$ (hrs) as discussed earlier. The input data for the carbonization processing analysis up to 15 hours is given in Table 6. The data generated in that run was stored in two tapes, SAVE = SAVE 1 and RESTRT = RSTRT 1. These two tapes are called to be used in the next run for conducting the subsequent processing analysis for $15 \le T \le 30$ (hours). The input data used for this analysis is given in Table 7. Similar data sets were made for carbonization analysis using other two sets of porosity (.55, .7), density (.065, .04)

TABLE 1

PROBLEMS SOLVED FOR ILLUSTRATING THE USE OF PEM COMPUTER CODE

Case	Problem	T_{Start}	T_{End}	Porosity	Density
1	Impregnation*	0	40 (Minutes)	.31	N/A
2	Carbonization	0 15	15 (Hrs) 30	.31	.1
3	Carbonization	0 15	15 30	.55	.0625
4	Carbonization	0 15	15 30	.7	.04
5	Graphitization	0	30	.11	.073

*Problems for impregnation have been solved in both rectangular and cylindrical coordinates. In all other cases (2-5), only rectangular coordinates have been used.

In Appendix A, the user instructions are given for the first four models. The input data and the results for a number of examples follow .

The problems solved for illustrating the use of the PEM computer code are given in Table 1. The preform and the processing can dimensions for different processes are given in Figures 3, 6 and 7. The PEM has been used to study the impregnation, the carbonization and the graphitization analyses. For each case, the finite element model and the relevant boundary/initial conditions are described separately. The thermochemical and physical properties of the billet preform and the liquid pitch are provided by SAI [5]. In modeling the billet two dimensional Cartesian coordinates, XZ, have been considered. The impregnation and the graphitization analyses are conducted for one set of porous medium porosity and density values. The carbonization analysis is done for three cases of porosity and density of the preform. The computer program was run for 15 time steps each time and the restart capability was used for the 30 hour carbonization analysis. In the first run, i.e. $0 \leq$ time ≤ 15 hours, the output was stored for its usage in the second run which is from 15 hours to 30 hours. All the results obtained during execution of these programs were stored for obtaining contour plots.

In the finite element modeling of impregnation process, Darcy's law for the flow of compressible fluid through porous media has been used. The effect of an external applied pressure has been considered and that of the capillary pressure has been ignored. Also, the time taken in pouring the fluid in the impregnation vessel has been assumed negligible. Figure 3 shows the billet finite element grid with relevant boundary conditions. Because of the geometric symmetry a quarter of the billet has been considered for finite element analysis. Thus, the following boundary and initial conditions were employed:

As shown in Figure 1a, the PEM Code has the following capabilities [1]:

1. Impregnation: This code is based upon Darcy's law of flow of compressible fluids through a porous media. The input parameters required for this analysis are given on page 8. Pressure boundary conditions are assigned. The effect of mechanical or capillary pressure can be studied separately. The present model does not account for the combined effect of capillary and mechanical pressure conditions.

2. Carbonization: This is the most involved process in the PEM and requires a unified treatment of the transfer of thermal energy by considering heat transfer, fluid motion and thermochemical reactions. Darcy's formulation has been utilized in developing this part of the code.

3. Graphitization: This capability of the PEM code is based upon the heat conduction in the billet including the influence of internal heat generation due to the carbonization and graphitization during processing.

4. Postprocessor: This code enables the user to obtain the results of different parameters in the form of contour plots.

5. TEMP3: This code has the capability to synthesize the thermal conductivity matrix [k] and the diffusion matrix [D] for a 3D composite given the similar properties for the constituents of the composite.

6. GRAPH: The degree of graphitization of the material in processing at any point of time can be estimated by using this model.

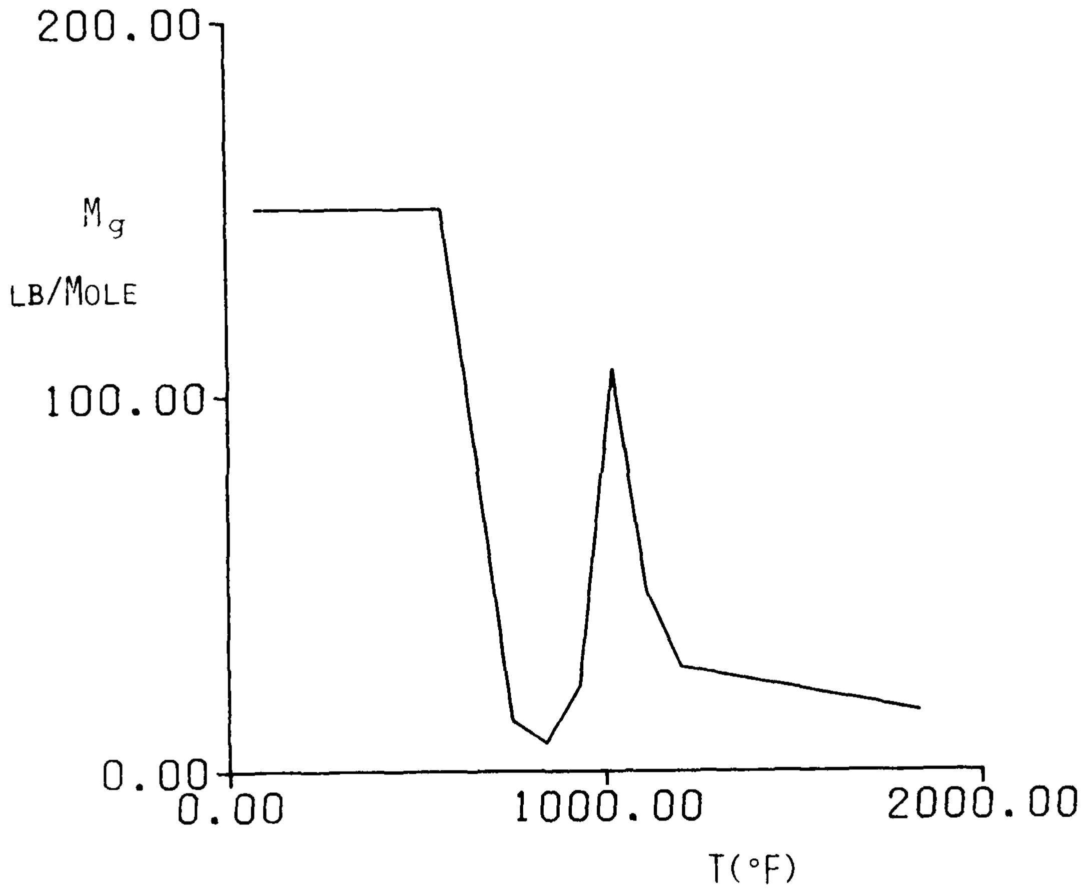


Figure 10. Gas Molecular Weight M_g Versus Temperature T.

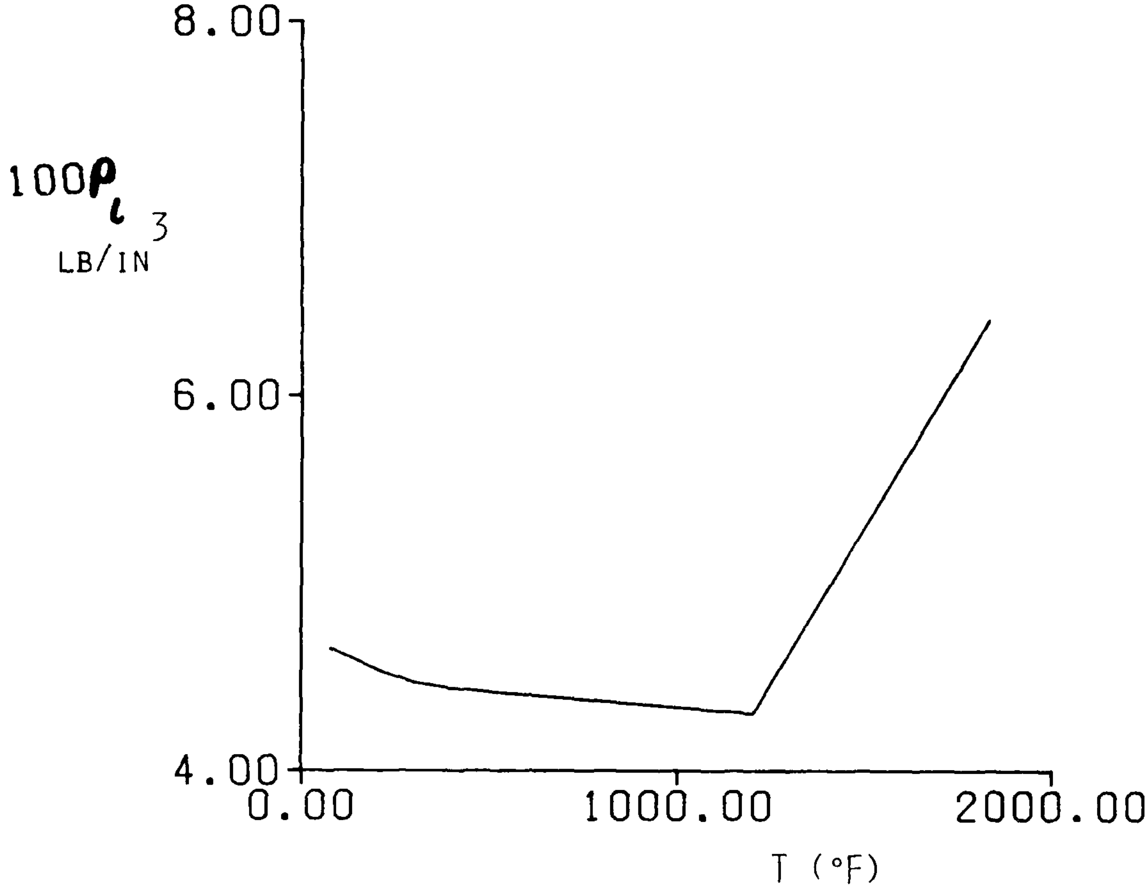


Figure 11. Liquid Pitch Density ρ_ℓ Versus Temperature T.

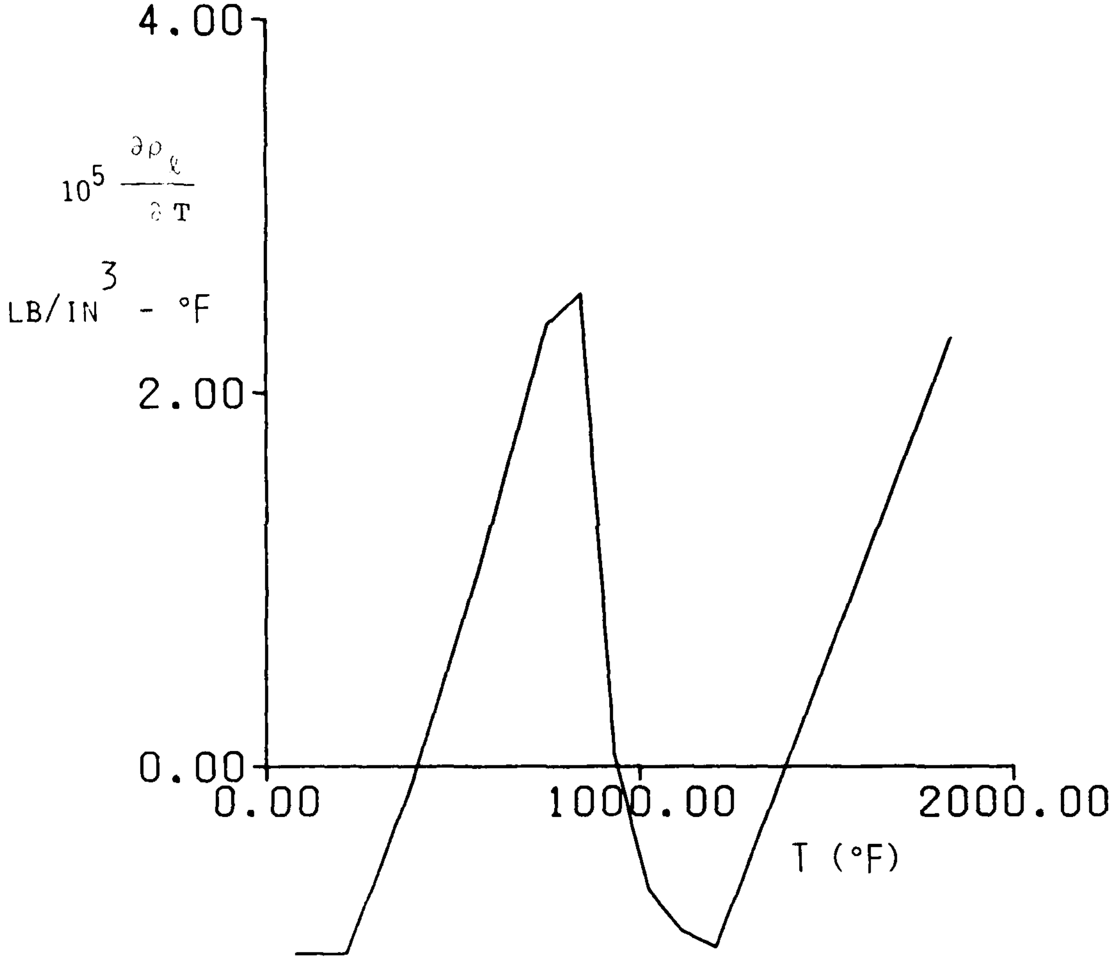


Figure 12. Rate of Change of Pitch Density with Temperature $\frac{\partial \rho_\ell}{\partial T}$ Versus Temperature T(°F).

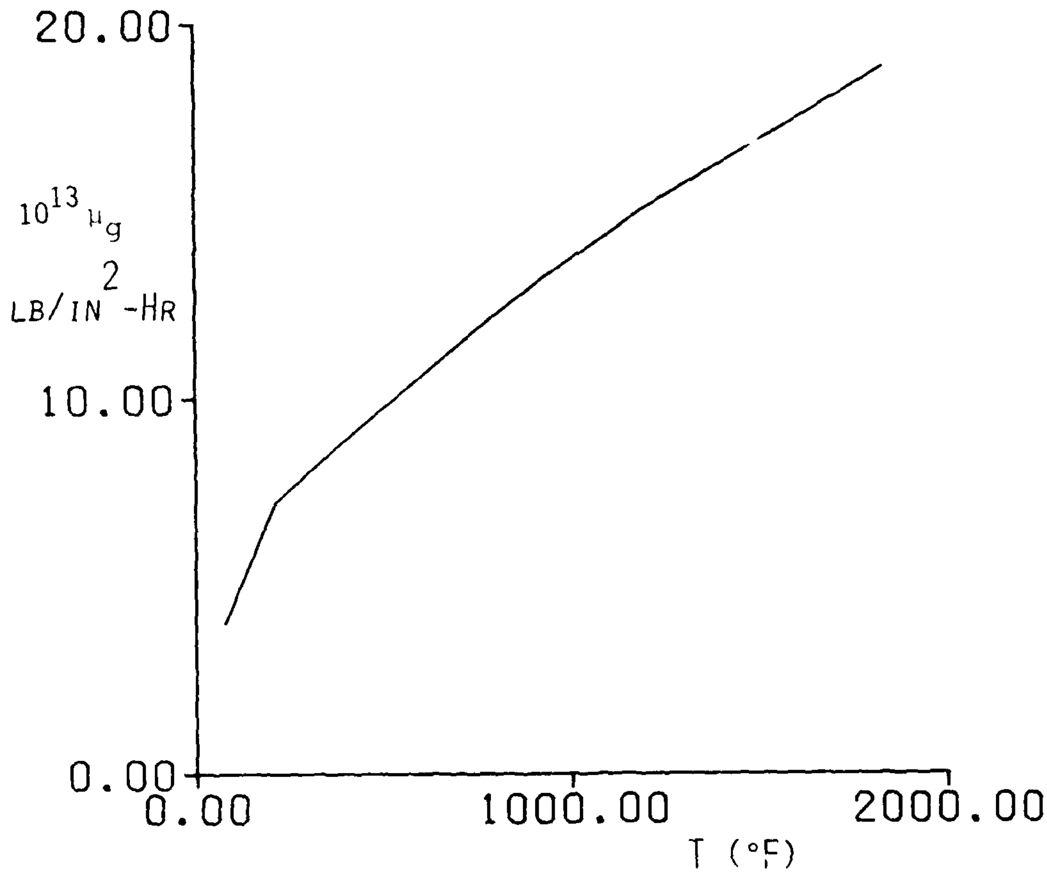


Figure 13. Gas Viscosity μ_g Versus Temperature T.

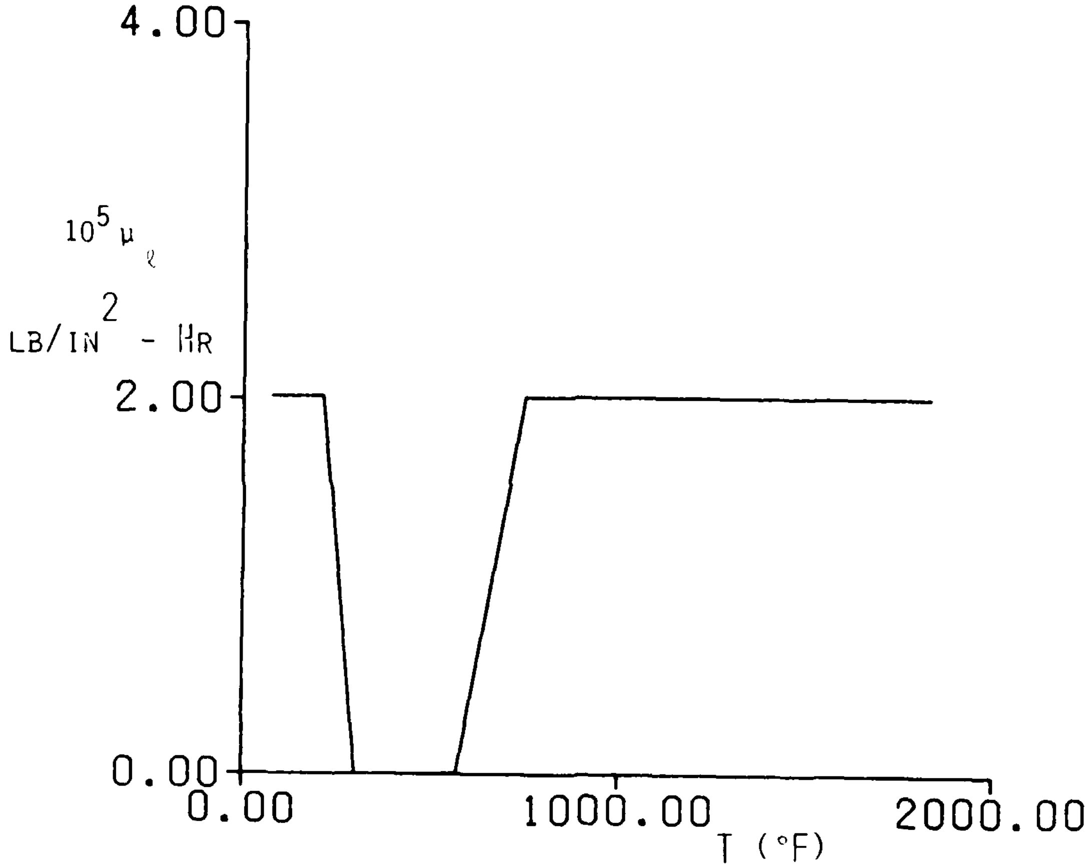


Figure 14. Liquid Pitch Viscosity μ_ℓ Versus Temperature T.

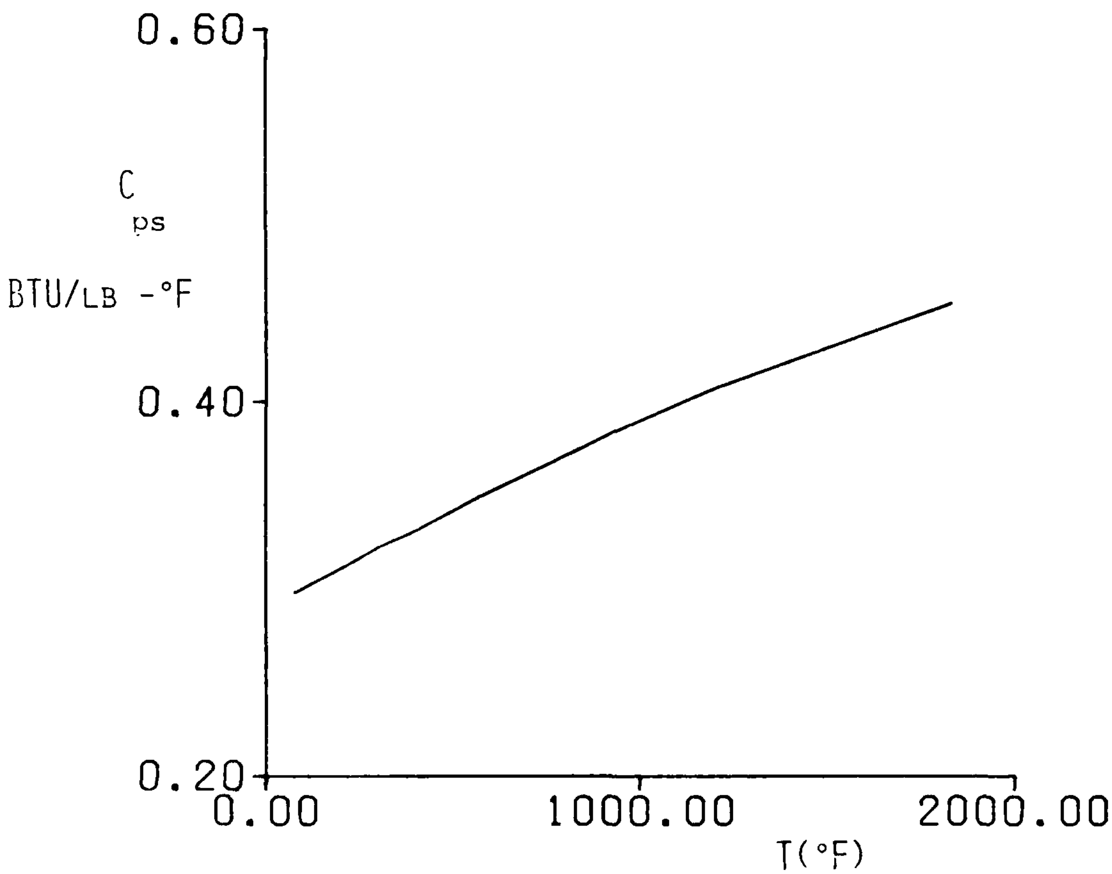


Figure 15. Yarn or Filler Specific Heat C_{ps} Versus Temperature T.

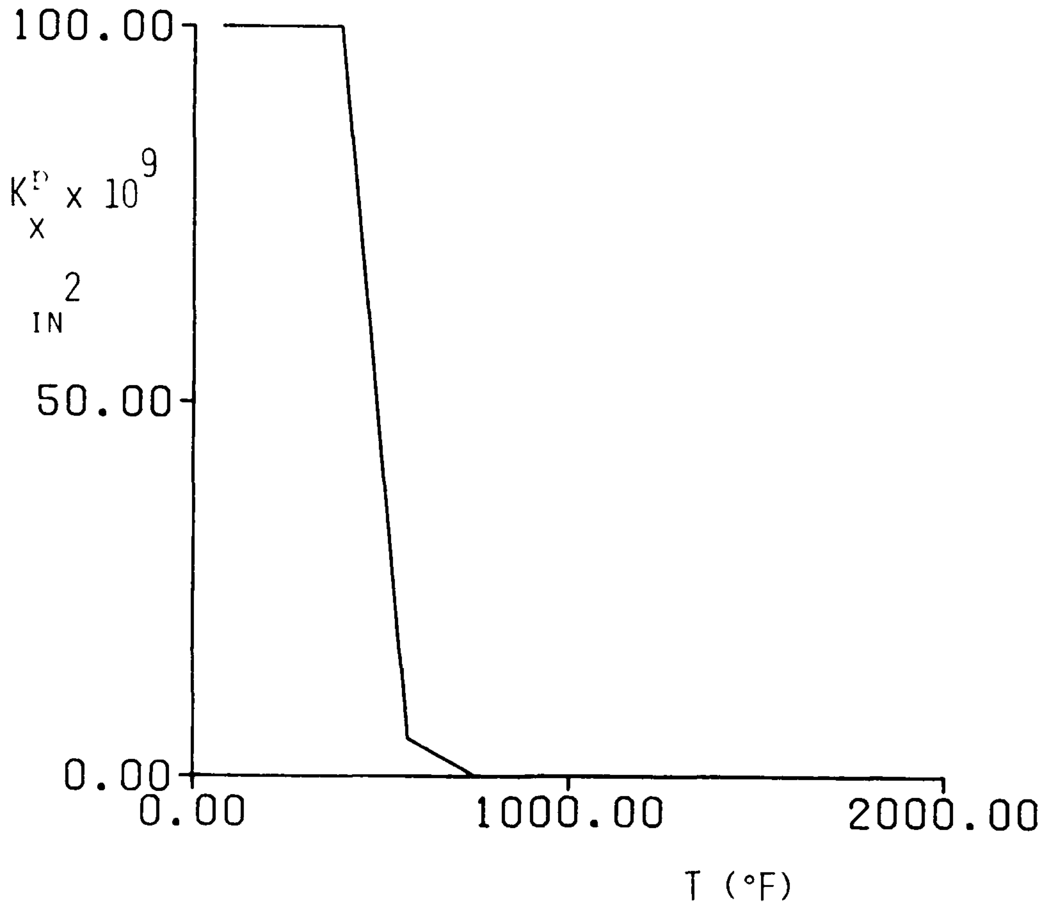


Figure 16. Liquid Permeability Component K^p_x Versus Temperature T.

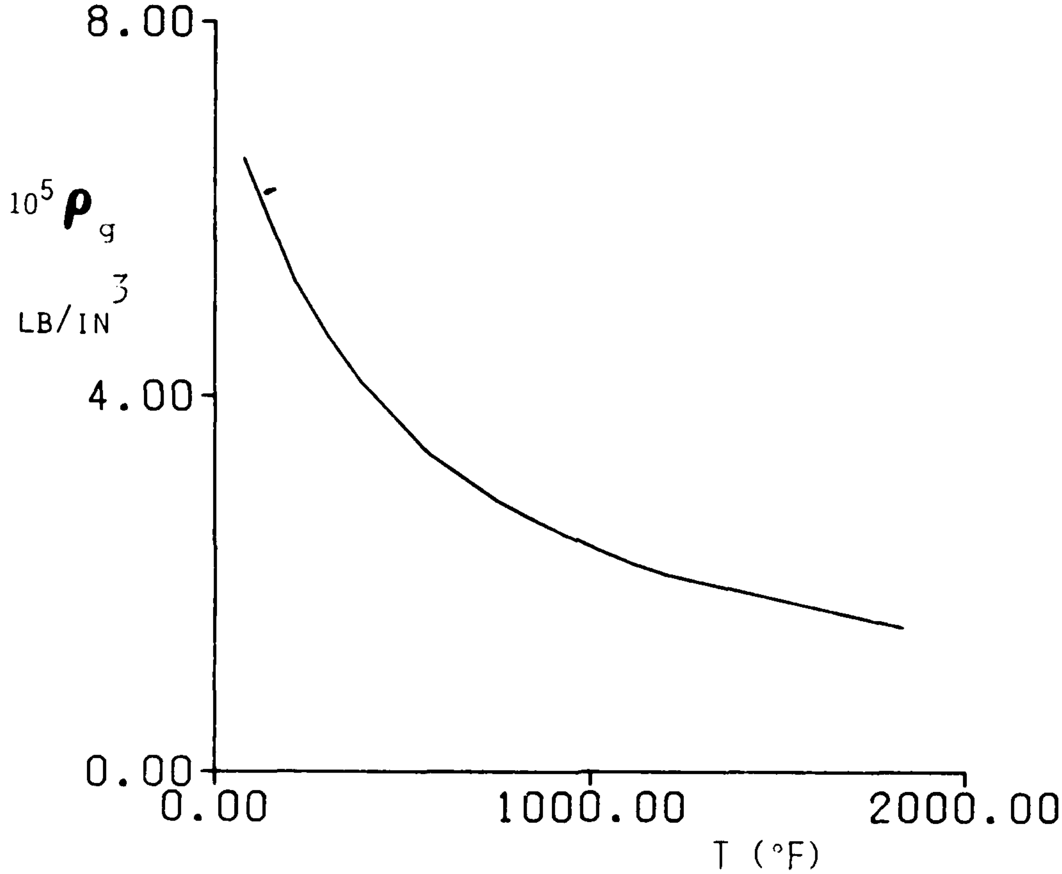


Figure 17. Gas Density ρ_g Versus Temperature T.

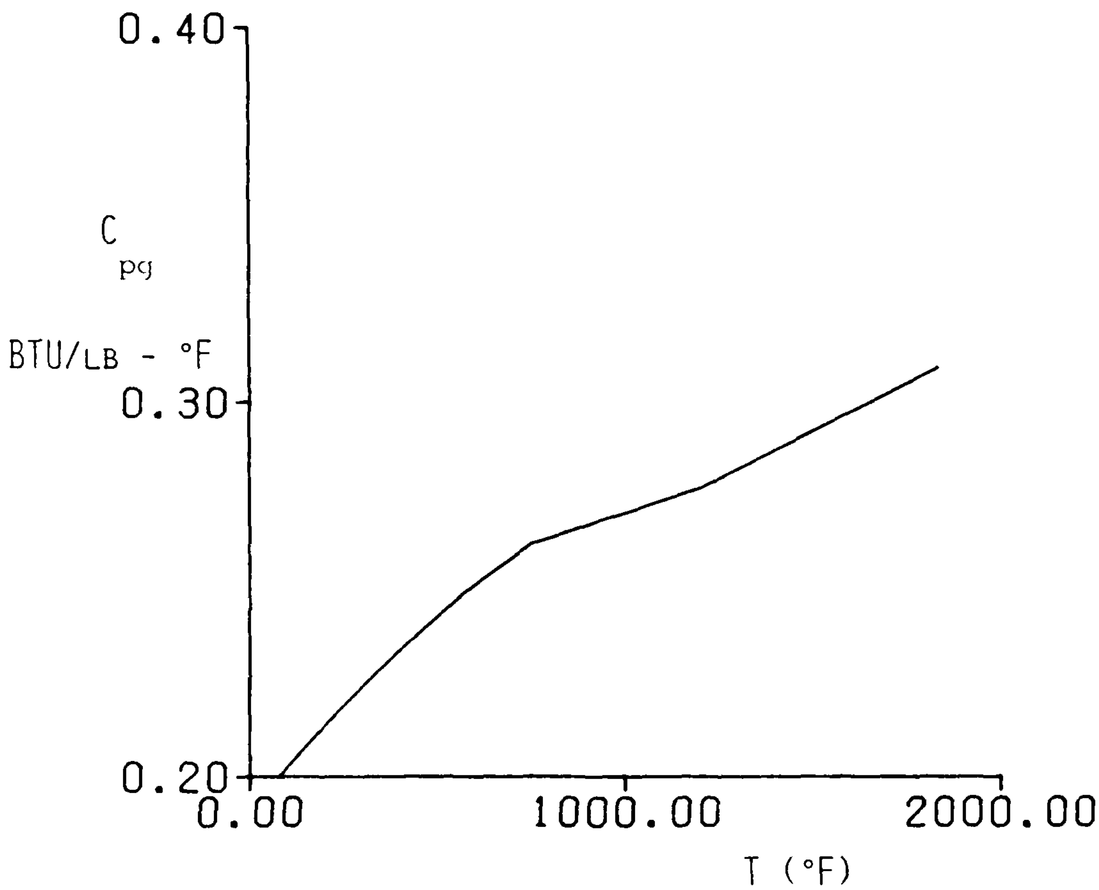


Figure 18. Gas Specific Heat C_{pg} Versus Temperature T.

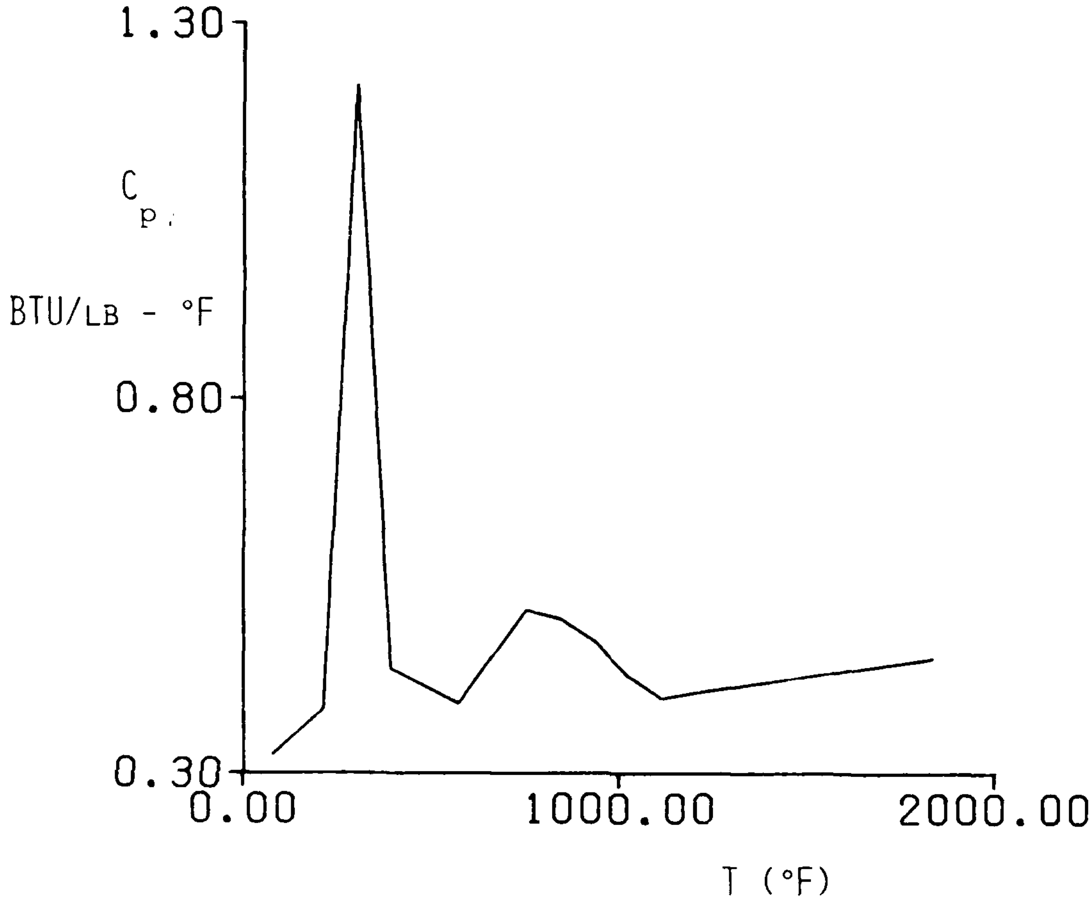


Figure 19. Liquid Pitch Specific Heat $C_{p\ell}$ Versus Temperature T.

TABLE 4

SOLID PREFORM MATERIAL PROPERTY TABLE
CORRESPONDING TO THE INPUT DATA QUANTITIES GIVEN ON PAGE 21 i.e.

$T,\ K_{MM},\ K_{NN},\ M_g,\ \rho_\ell,\ \frac{\partial \rho_\ell}{\partial T}$ Format (7F10.0)

[illegible], [illegible], $C_{p\ell}$, K_x^{p*}, K_z^{p*} Format (10X, 5F10.0)

k_g, C_{pg}, C_p Format (10X, 4F10.0)

.5370E+03	.3320E+01	.3590E+01	.1500E+030.		.4650E-01-.1004E-04
	.4020E-12	.2013E-04	.2300E+00	.1000E-06	.1000E-06
	.6538E-04	.2000E+00	.3250E+00		
.6720E+03	.2890E+01	.2990E+01	.1500E+030.		.4530E-01-.1004E-04
	.7247E-12	.2013E-04	.2630E+00	.1000E-06	.1000E-06
	.5236E-04	.2150E+00	.3850E+00		
.7620E+03	.2720E+01	.2810E+01	.1500E+030.		.4470E-01-.5530E-05
	.8052E-12	.2416E-08	.2810E+00	.1000E-06	.1000E-06
	.4637E-04	.2240E+00	.1217E+01		
.8520E+03	.2650E+01	.2800E+01	.1500E+030.		.4440E-01-.7190E-06
	.8857E-12	.2536E-08	.2980E+00	.1000E-06	.1000E-06
	.4136E-04	.2330E+00	.4390E+00		
.1032E+04	.2444E+01	.2545E+01	.1500E+030.		.4410E-01 .1070E-04
	.1035E-11	.4429E-07	.3275E+00	.5000E-07	.5000E-07
	.3379E-04	.2489E+00	.3926E+00		
.1212E+04	.2290E+01	.2360E+01	.1360E+020.		.4380E-01 .2360E-04
	.1188E-11	.2013E-04	.3530E+00	.1000E-08	.1000E-08
	.2880E-04	.2620E+00	.5170E+00		
.1302E+04	.2330E+01	.2410E+01	.7500E+010.		.4365E-01 .2530E-04
	.1260E-11	.2013E-04	.3640E+00	.1000E-08	.1000E-08
	.2691E-04	.2650E+00	.5050E+00		
.1392E+04	.2480E+01	.2580E+01	.2280E+020.		.4350E-01 .6630E-06
	.1329E-11	.2013E-04	.3750E+00	.1000E-08	.1000E-08
	.2521E-04	.2690E+00	.4760E+00		
.1492E+04	.2880E+01	.3000E+01	.1070E+030.		.4335E-01-.6590E-05
	.1389E-11	.2013E-04	.3860E+00	.1000E-08	.1000E-08
	.2356E-04	.2710E+00	.4300E+00		
.1572E+04	.2960E+01	.3080E+01	.4770E+020.		.4320E-01-.8800E-05
	.1449E-11	.2013E-04	.3980E+00	.1000E-08	.1000E-08
	.2210E-04	.2740E+00	.4000E+00		
.1652E+04	.2866E+01	.2985E+01	.2780E+020.		.4305E-01-.9680E-05
	.1514E-11	.2013E-04	.4086E+00	.1000E-08	.1000E-08
	.2090E-04	.2770E+00	.4077E+00		
.2292E+04	.2360E+01	.2450E+01	.1600E+020.		.6400E-01 .2290E-04
	.1884E-11	.2013E-04	.4530E+00	.1000E-08	.1000E-08
	.1538E-04	.3090E+00	.4530E+00		

Curing time table for carbonization is:

Time, Temp. Format (8F10.2)

0.00	[illegible]37.00	[illegible].00	1121.00	27.00	1571.00	34.00	1931.
[illegible]5.00	[illegible]51.00	[illegible].00	1391.00				

In these input tables, the temperature T is given in °R, whereas in figures we have used °F. The output contours are in °C.

*Values of K_x^p, K_z^p considered for three different cases of carbonization analysis investigated in this work are given on page 56.

TABLE 5

PERMEABILITY (K^p) VALUES CONSIDERED FOR DIFFERENT CASES, $K^p = K^p_x = K^p_z$

Temp. (°F)	Porosity=.31 Density=.1 $K^p(in^2)$	Porosity=.55 Density=.0625 $K^p(in^2)$	Porosity=.7 Density=.04 $K^p(in^2)$
77	.1E-09	.1E-07	.1E-06
212	.1E-09	.1E-07	.1E-06
302	.1E-09	.1E-07	.1E-06
392	.1E-09	.1E-07	.1E-06
572	.5E-10	.5E-08	.5E-07
752	.1E-11	.1E-09	.1E-08
842	.1E-11	.1E-09	.1E-08
932	.1E-11	.1E-09	.1E-08
1022	.1E-11	.1E-09	.1E-08
1112	.1E-11	.1E-09	.1E-08
1202	.1E-11	.1E-09	.1E-08
1832	.1E-11	.1E-09	.1E-08

The data for porosity = .31 and density = 0.1 was from [5], whereas, for other two cases it was assumed.

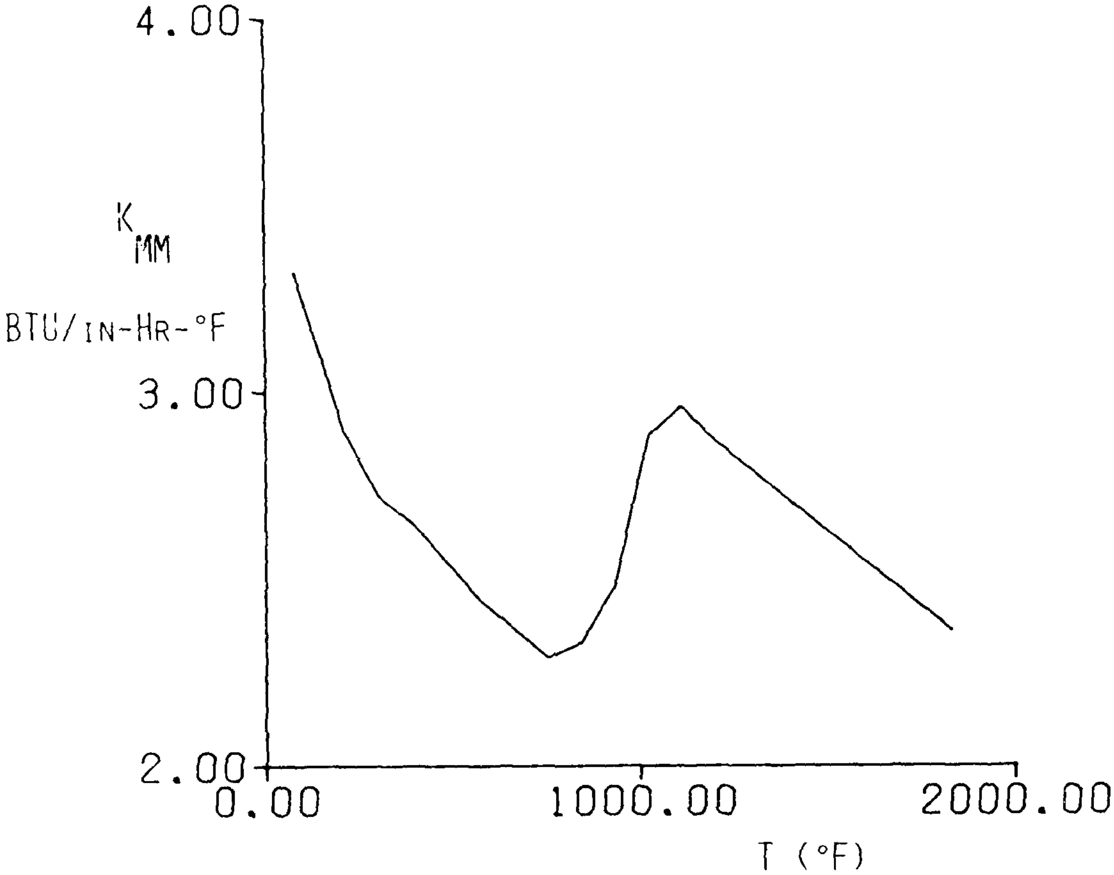


Figure 20. Solid Thermal Conductivity K_{MM} Versus Temperature T.

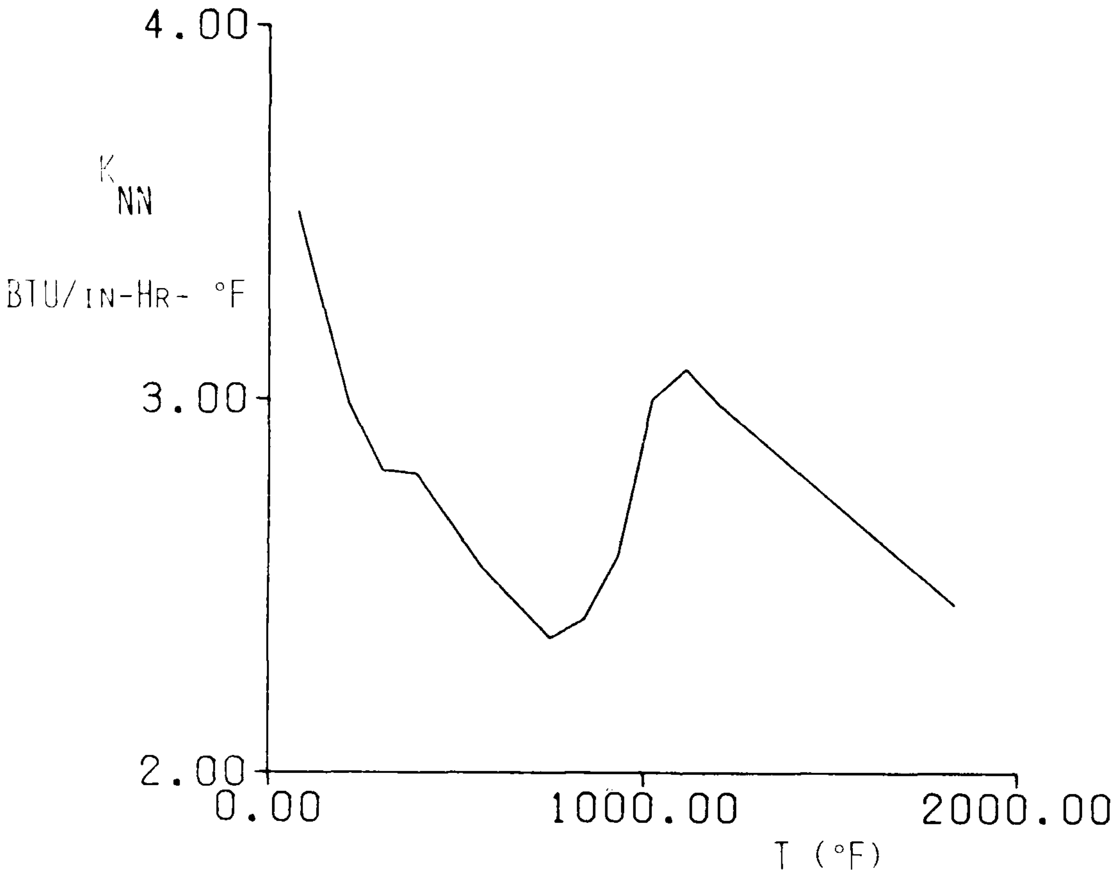


Figure 21. Solid Thermal Conductivity K_{NN} Versus Temperature T.

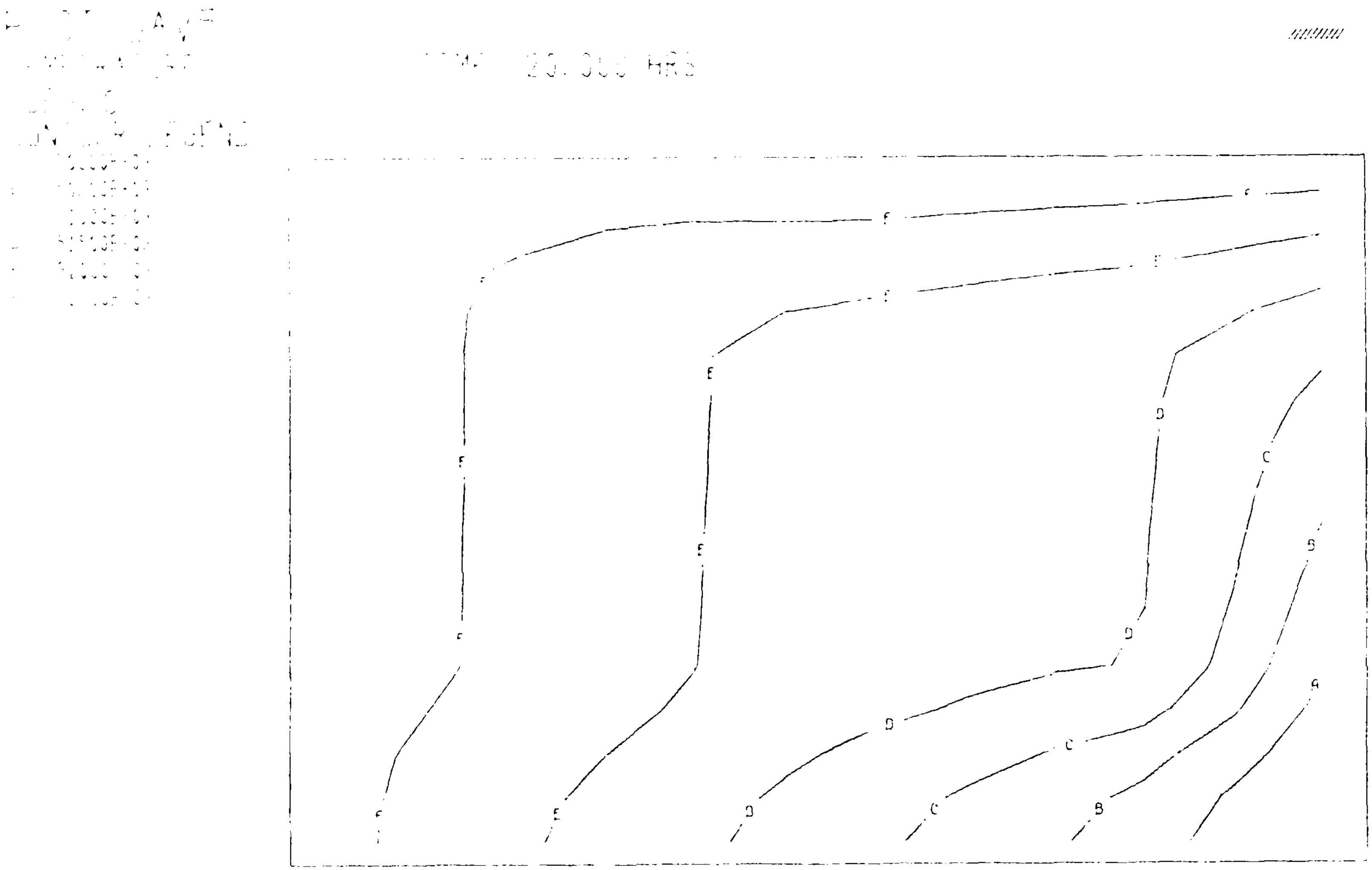


Figure 29. Temperature Contours in Carbonization Analysis.

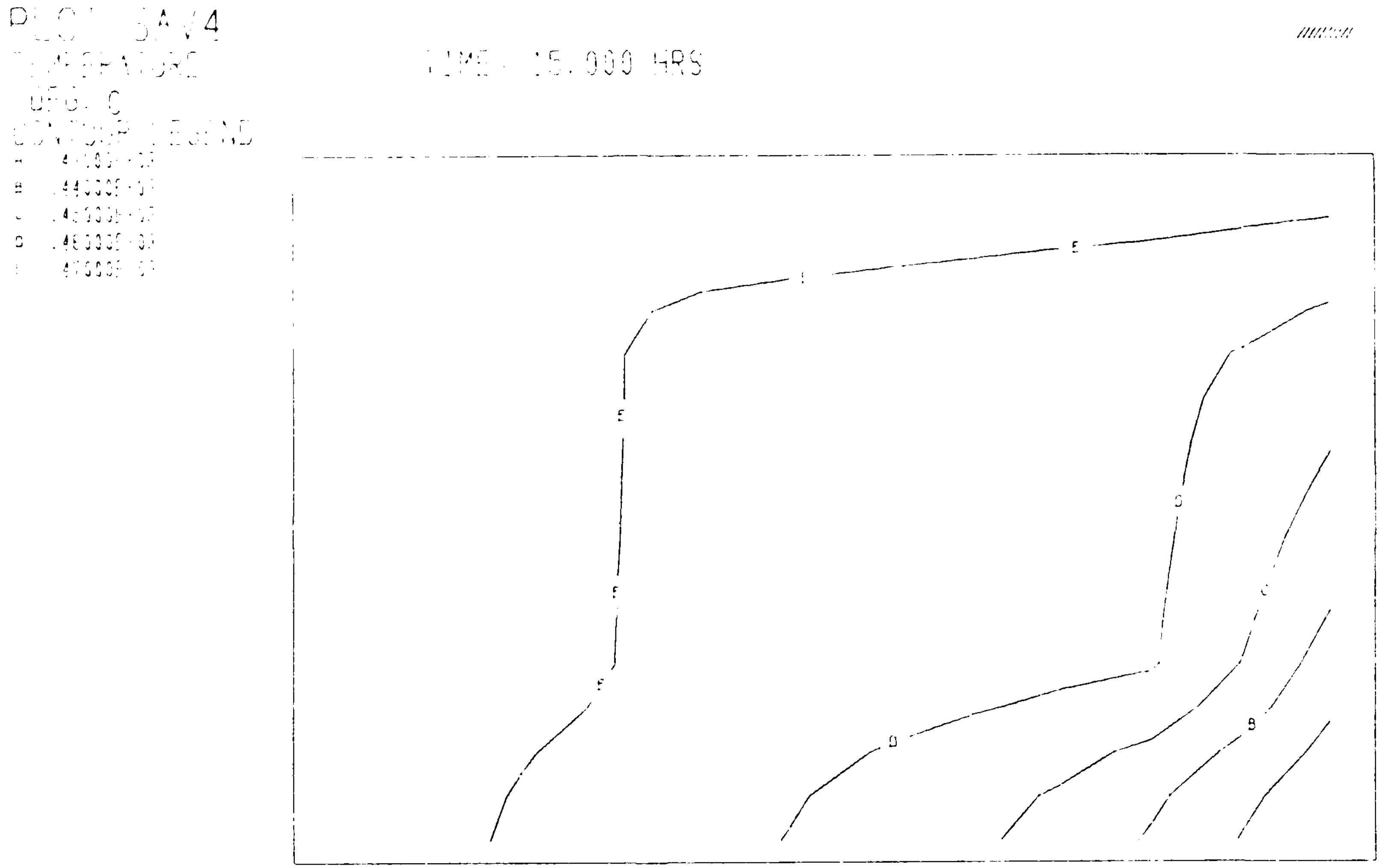


Figure 28. Temperature Contours in Carbonization Analysis.

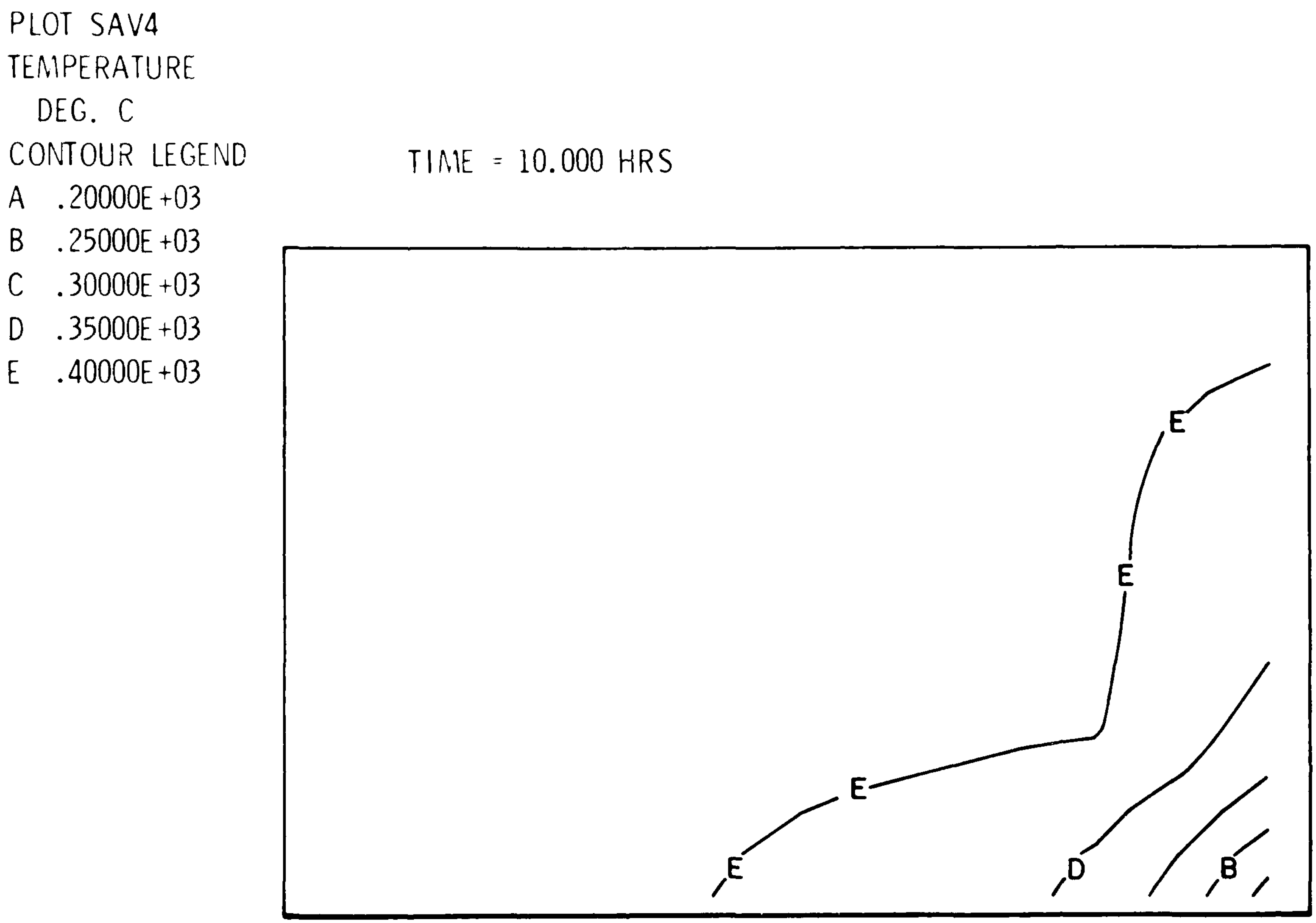


Figure 27. Temperature Contours in Carbonization Analysis.

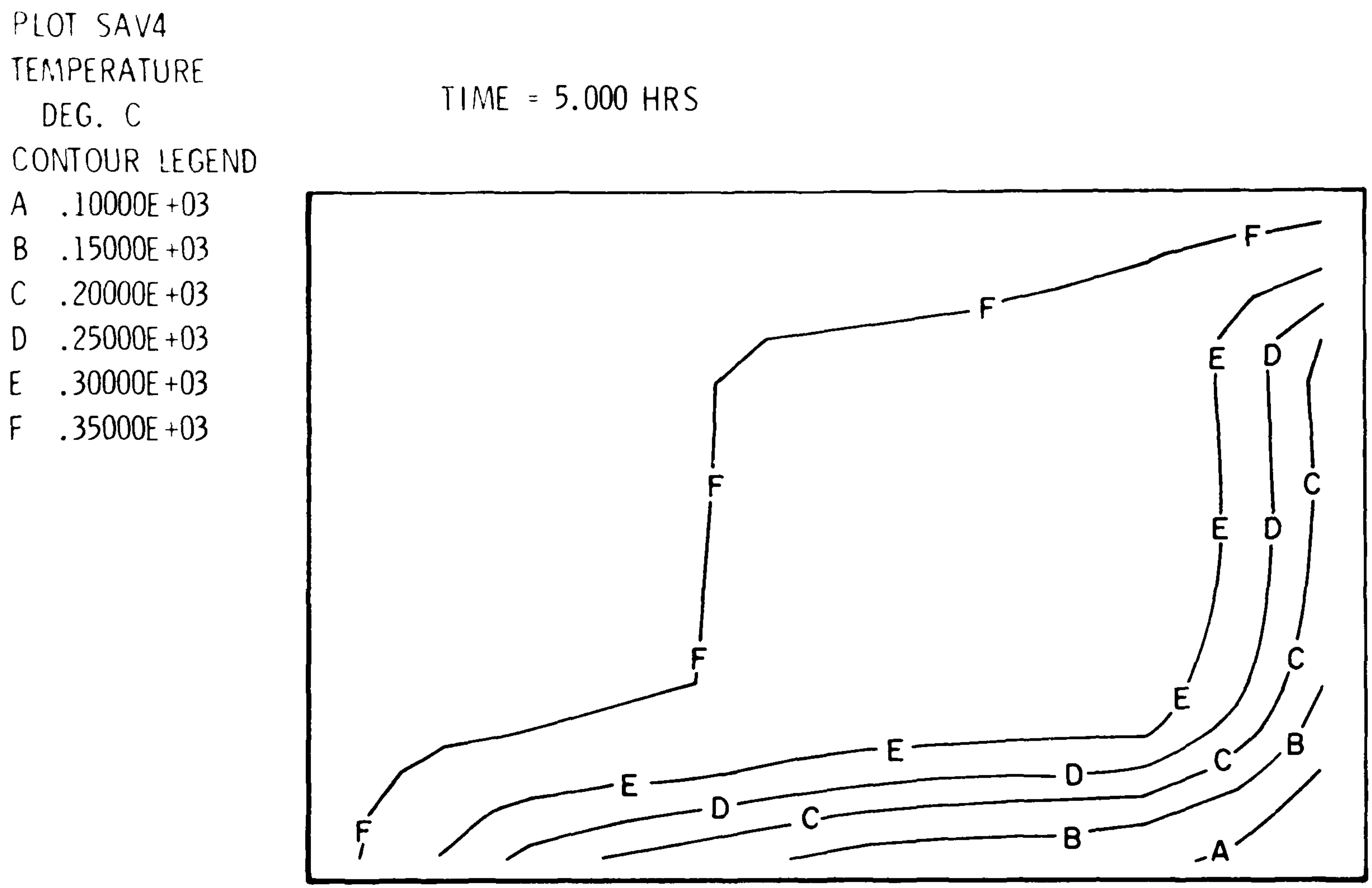


Figure 26. Temperature Contours in Carbonization Analysis.

CARBONIZATION ANALYSIS OUTPUT

PREFORM POROSITY = 0.31

PREFORM DENSITY = 0.1

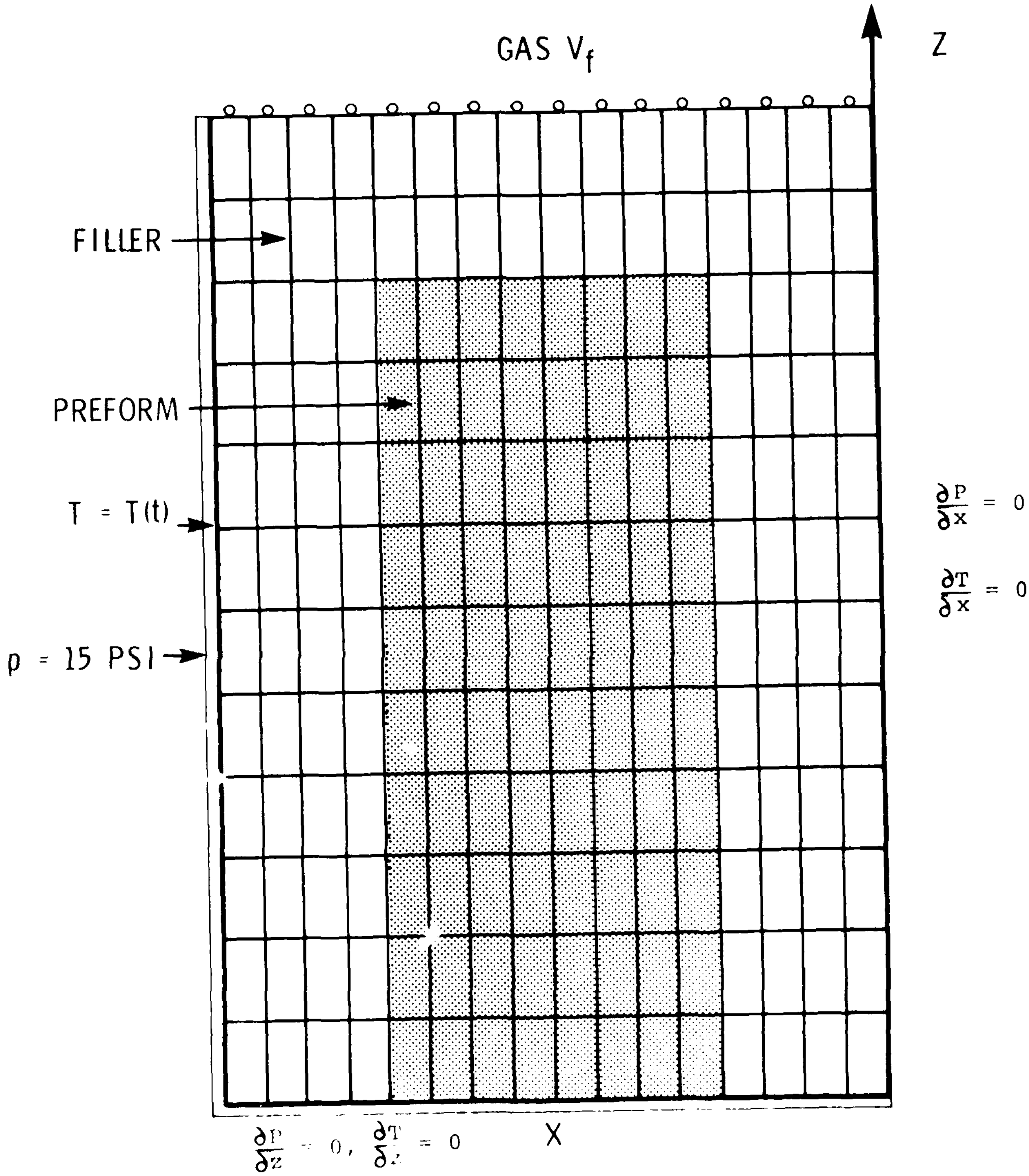


Figure 25. Carbonization Boundary Conditions.

In the input of Table 6, the processing analysis was done up to 15 hours. The data generated in that run was stored in two tapes, SAVE = SAVE 1 and RESTRT = RESTRT 1. These two tapes are attached to use in the next run to conduct the processing analysis from 15 hours to 30 hours. The input for this analysis is given in Table 7.

The aforementioned data sets are given for a billet with porosity = 0.31, density = 0.1 and corresponding values of permeability from Table 5. Similar data sets with other two values of porosity (0.55, 0.7), density (0.065, 0.04) and permeability (Table 5) were used to conduct carbonization analysis. The contour plots of significant parameters for all the three cases are given in the following section. In the plotting run for these contour plots, we have used the automatic scale choice option, and for that reason, the figures are not consistent with the finite element grid axis shown in Figure 7. Contour figures are consistent with the billet axis and boundary conditions shown in Figure 25.

TABLE 7

IMAGES OF DATA FOR CARBONIZATION ANALYSIS FOR TIME T=15 TO T=30 HOURS

```
 ----------------------------------------------------------------------------------
 1         10        20        30        40        50        60        70        80
 ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?
 ----------------------------------------------------------------------------------
 1-CARBONIZATION OF EXAMPLE PROBLEM 8X12 BILLET
 2-    1    2    0    1    1    0    6    1    2
 3- 15.      30.0      1.0       100.           1    15   0    2
 4-    3    1    2    3
 5-    1    1    1   17    1    1 1.0       1.0
 6-    1   17    1   17   13    1 1.        1.
 7-    1    1    1   17    1    0 15.       15.
 8-    1   17    1   17   13    0 15.       15.
 9-    2    1   13   17   13    0 15.       15.
10-    3    1   13   17   13    0 0.01      0.01
11-0.4       0.01      1.10      0.026446  0.2674
12-18543.72  0.        0.        0.        5.00308E05.00308E099338.03   18.0
13-1.57      1107.     143.      2500.
14-0.025     1273.     57.6      81000.
15-0.08      1255.4    153.0     0.
16-    1   12    1    35.2731E-071.0       0.
```

Cards 17 through 52 are the same as liquid pitch properties Table 3 page 42.

```
53-    2   12    0    31.27315-370.7       0.04
```

Cards 54 through 89 are the same as solid preform properties Table 4 on page 55.

```
90-    1    6
91-  0.      537.      0.        1121.     27.       1571.     34.       1931.
92-  35.     1931.     36.       1591.
93-END OF CASE
   :----:----:----:----:----:----:----:----:----:----:----:----:----:----:----:----:
```

TABLE 6

IMAGES OF DATA FOR CARBONIZATION ANALYSIS FOR TIME T=0 TO T=15 HOURS

```
 ----------------------------------------------------------------------------------
 1        10        20        30        40        50        60        70        80
 ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?
 ----------------------------------------------------------------------------------
1-CARBONIZATION OF EXAMPLE PROBLEM 8X12 BILLET                                    -
2-    1    0    0    1    1    0    6    1    2                                   -
3- 0.        15.0      1.0       100.          1    15   0    2                   -
4-    7    1    2    3                                                            -
5-   17   13   12             4  150                                              -
6-  1  1  0.       0.     17  1  8.     0.                              1         -
7- 17  1  0.       0.     17 13  0.     12.                             1         -
8- 17 17  8.      12.      1 13  0.     12.                             1         -
9-  1 13  0.      12.      1  1  0.     0.                              1         -
10- -1                                                                            -
11-    1    1   17    1   10                                                      -
12-    2    5   13    1   11                                                      -
13-    1    1    1   17    1    1 1.0      1.0                                    -
14-    1   17    1   17   13    1 1.       1.                                     -
15-    0    1    1   17    1    0 15.      15.                                    -
16-    2   17    1   17   13    0 15.      15.                                    -
17-    2    1   13   17   13    0 15.      15.                                    -
18-    3    1   13   17   13    0 0.01     0.01                                   -
19-                              537.      15.        0.01                        -
20-0.4       0.01      1.10      0.826446  0.2674                                 -
21-19543.70  0.        0.        0.        5.00308E095.00308E099338.03   18.0     -
22-0.570     1107.     193.      2500.                                            -
23-0.020     1273.     57.6      -1000.                                           -
24-0.08      1875.4    153.0     0.                                               -
25-    1   12    1   35.2731E-071.0        0.                                     -
```

Cards 26 through 61 are the same as liquid pitch properties Table 3 on page 42.

```
62-    2   12    0   35.2731E-070.7        0.04
```

Cards 63 through 98 are the same as solid preform properties Table 4 on page 55.

```
99-    1    6                                                                     -
100-   0.      537.      2.        1121.     27.       1571.     34.       1931.    -
101-   33.     1931.     36.       1391.                                            -
102-END OF CASE                                                                   -
    :----:----:----:----:----:----:----:----:----:----:----:----:----:----:----:----:
```

CARBONIZATION ANALYSES INPUT

The following material properties are common to both (Table 3) liquid pitch material property and (Table 4) solid preform material property.

1) Gas molecular weight M_g (Fig. #10)
2) Liquid pitch density ρ_ℓ (Fig. #11)
3) Rate of change of pitch density with respect to temperature $\frac{\partial \rho_\ell}{\partial T}$ (Fig. #12)
4) Gas viscosity μ_g (Fig. #13)
5) Liquid pitch viscosity μ_ℓ (Fig. 14)
6) Gas density ρ_g. (Fig. #17)
7) Gas specific heat C_{pg} (Fig. #18)
8) Liquid pitch specific heat C_{pl} (Fig. #19)

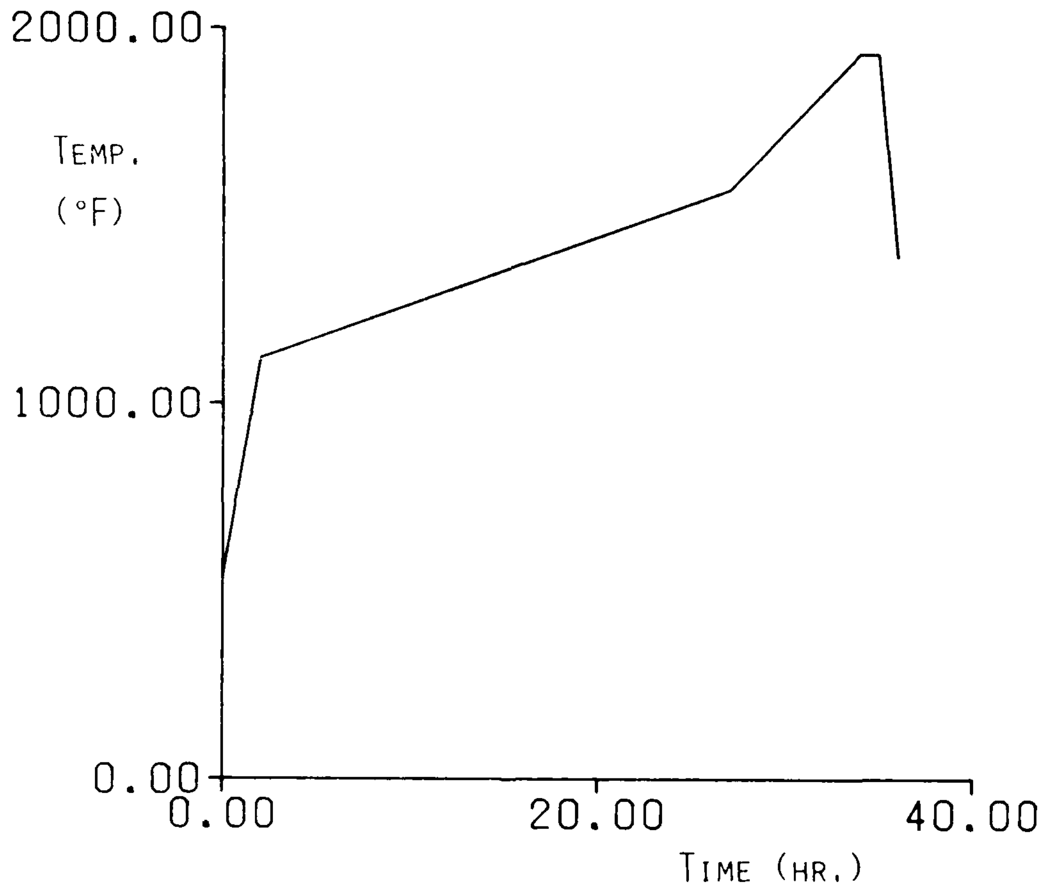


Figure 24. Carbonization Process Temperature - Time History.

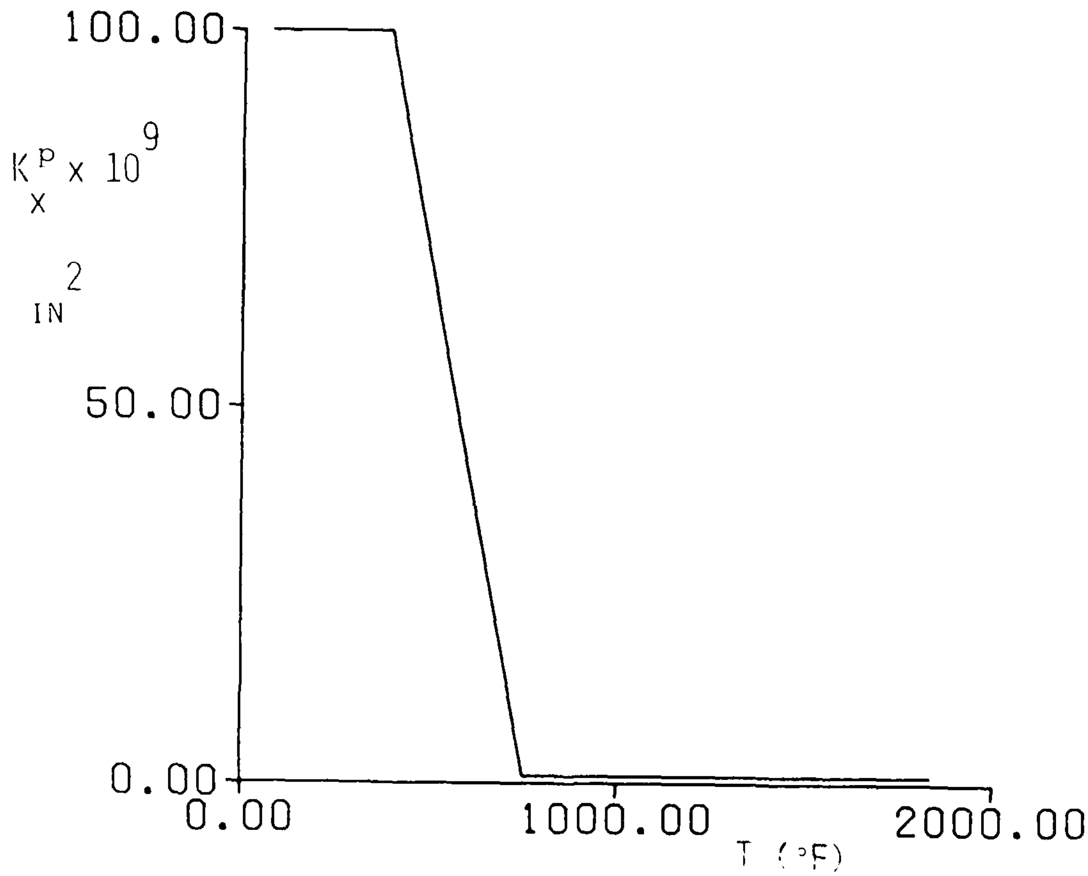


Figure 23. Solid Permeability K^p_x (or K^p_z) Versus Temperature.

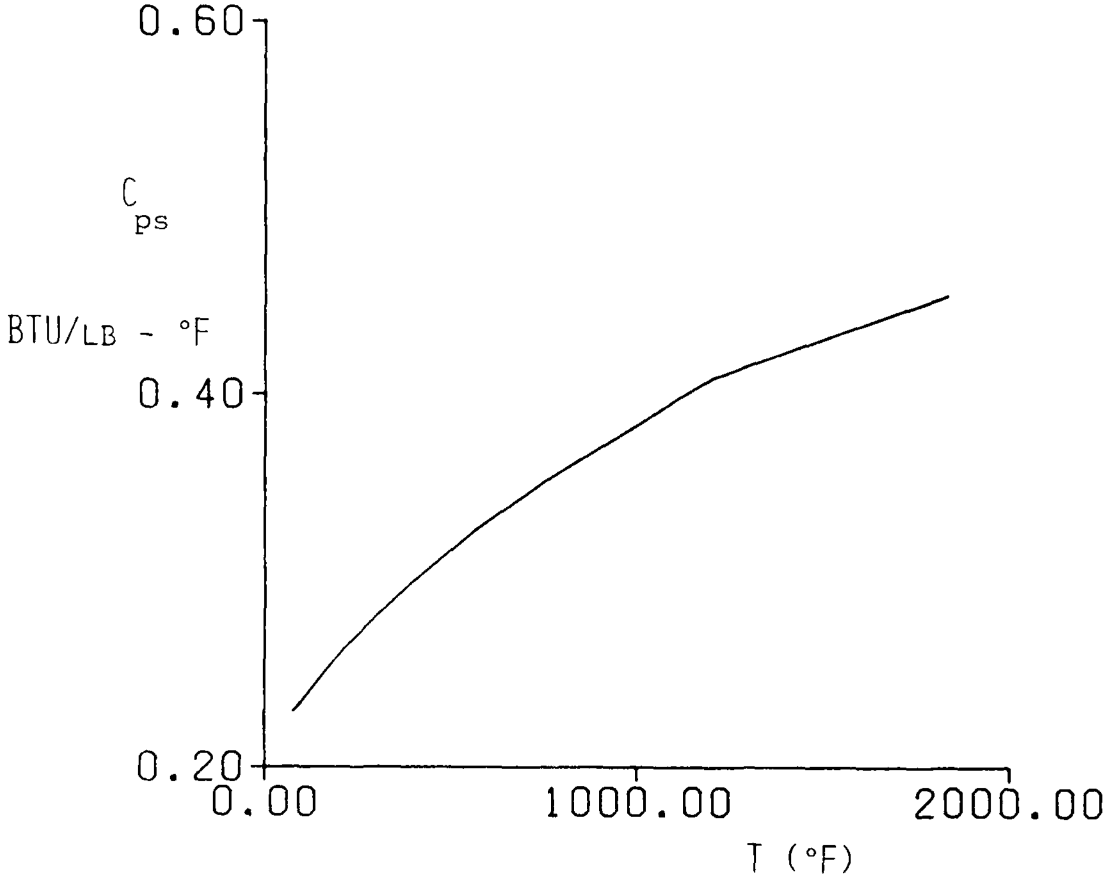


Figure 22. Yarn or Filler Specific Heat C_{ps} Versus Temperature T.

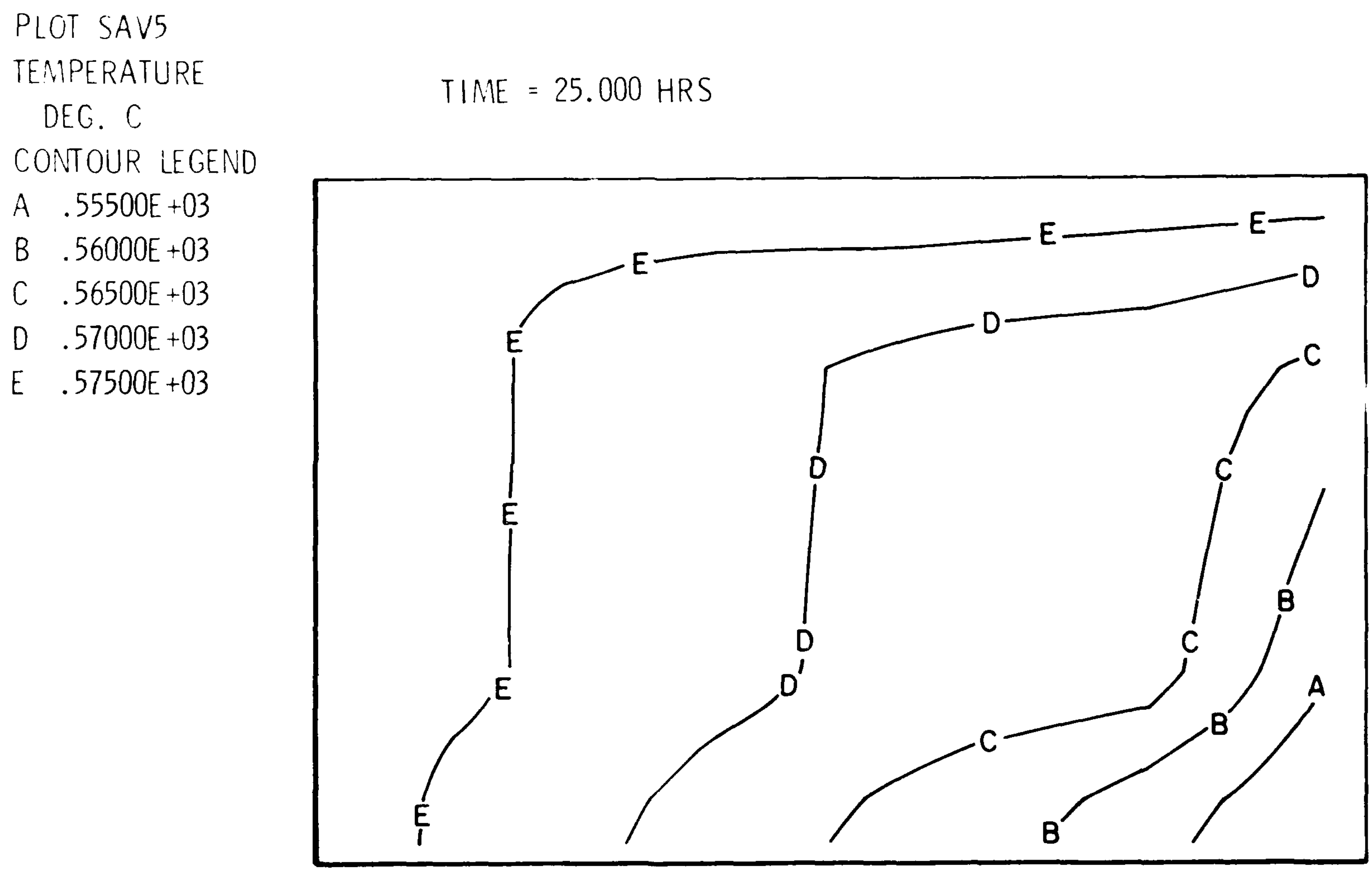


Figure 30. Temperature Contours in Carbonization Analysis.

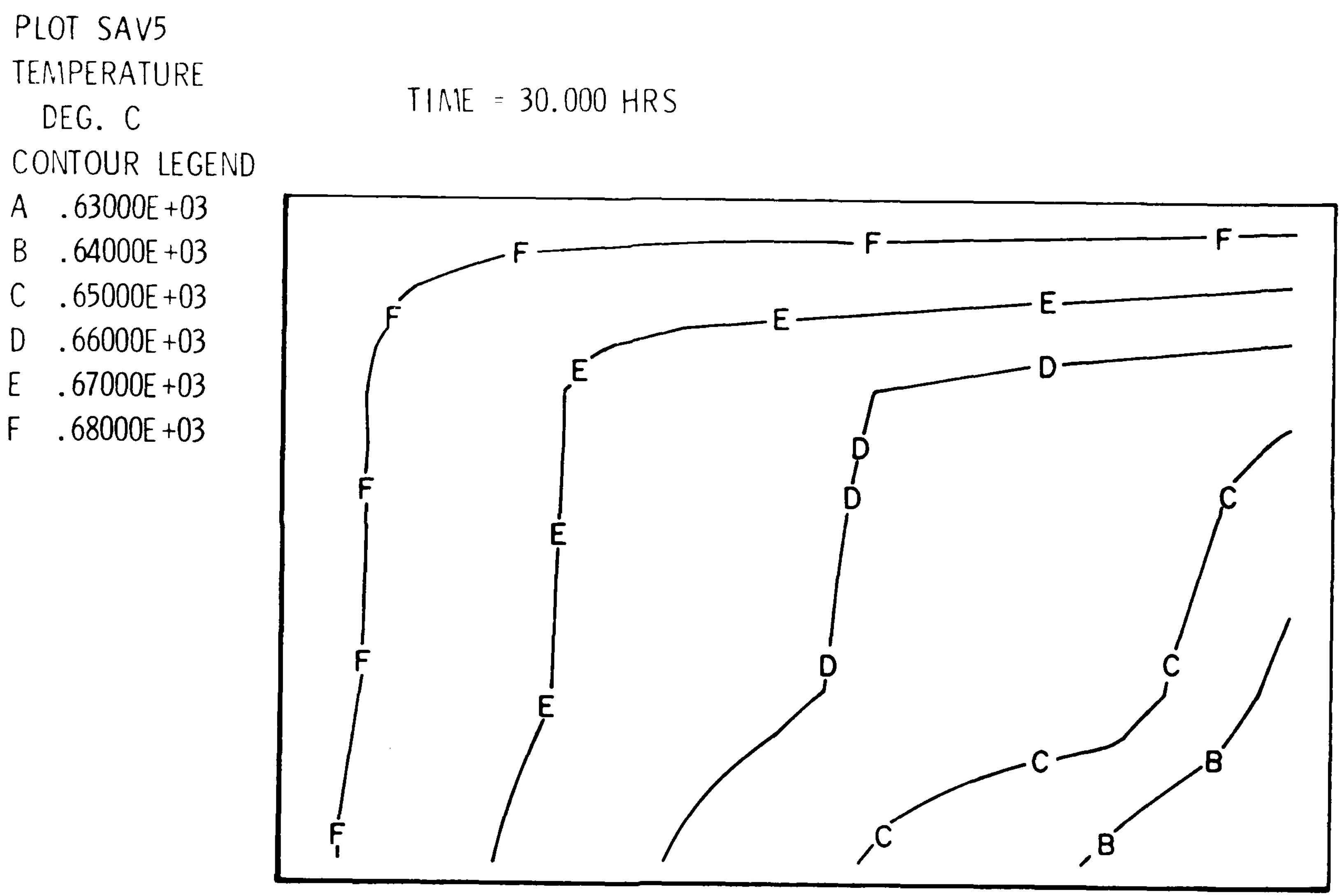


Figure 31. Temperature Contours in Carbonization Analysis.

PLOT SAV4
PRESSURE
PSI
CONTOUR LEGEND
A .20000E+02
B .30000E+02
C .40000E+02
D .50000E+02
E .60000E+02
F .70000E+02

TIME = 5.000 HRS

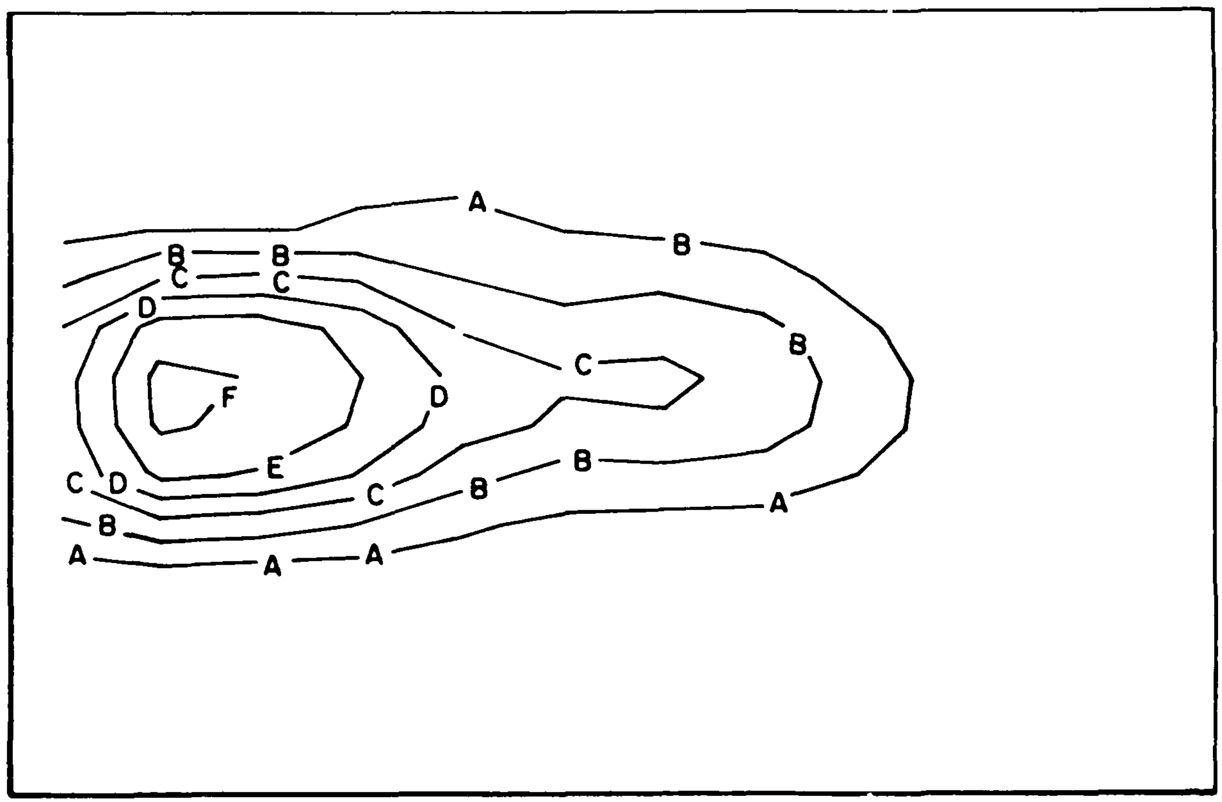


Figure 32. Pressure Contours for Carbonization Analysis.

PLOT SAV5
PRESSURE
PSI
CONTOUR LEGEND

A	.20000E+02
B	.30000E+02
C	.40000E+02
D	.50000E+02
E	.60000E+02

TIME = 30.000 HRS

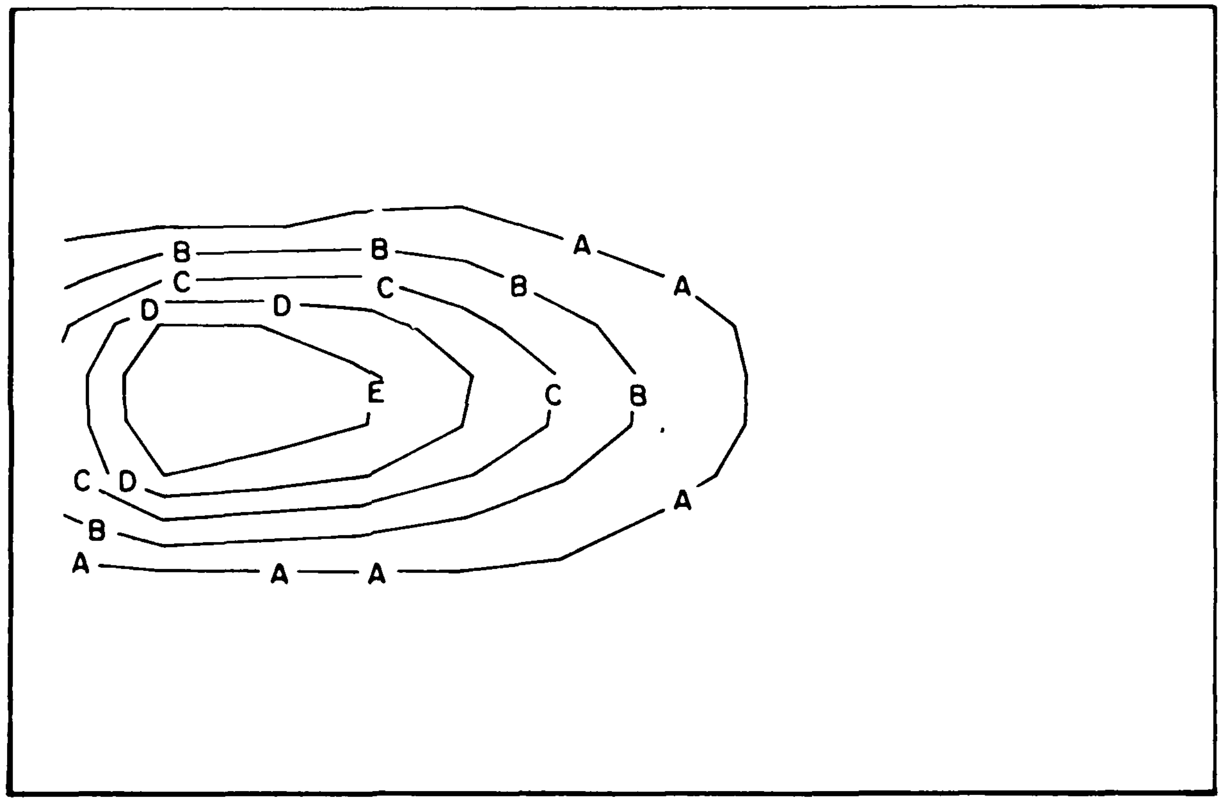


Figure 33. Pressure Contours for Carbonization Analysis.

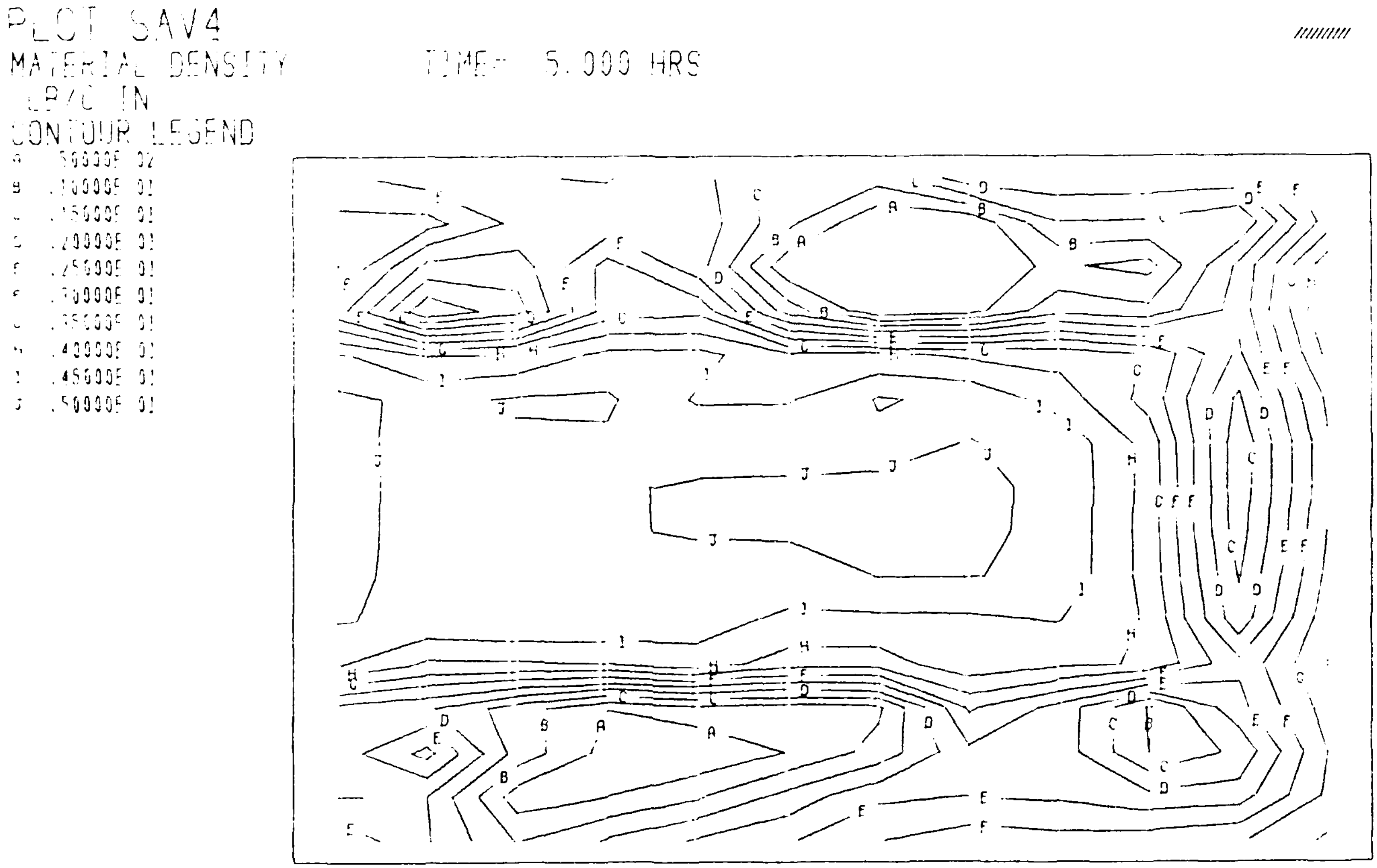


Figure 34. Material Density Contours in Carbonization Analysis.

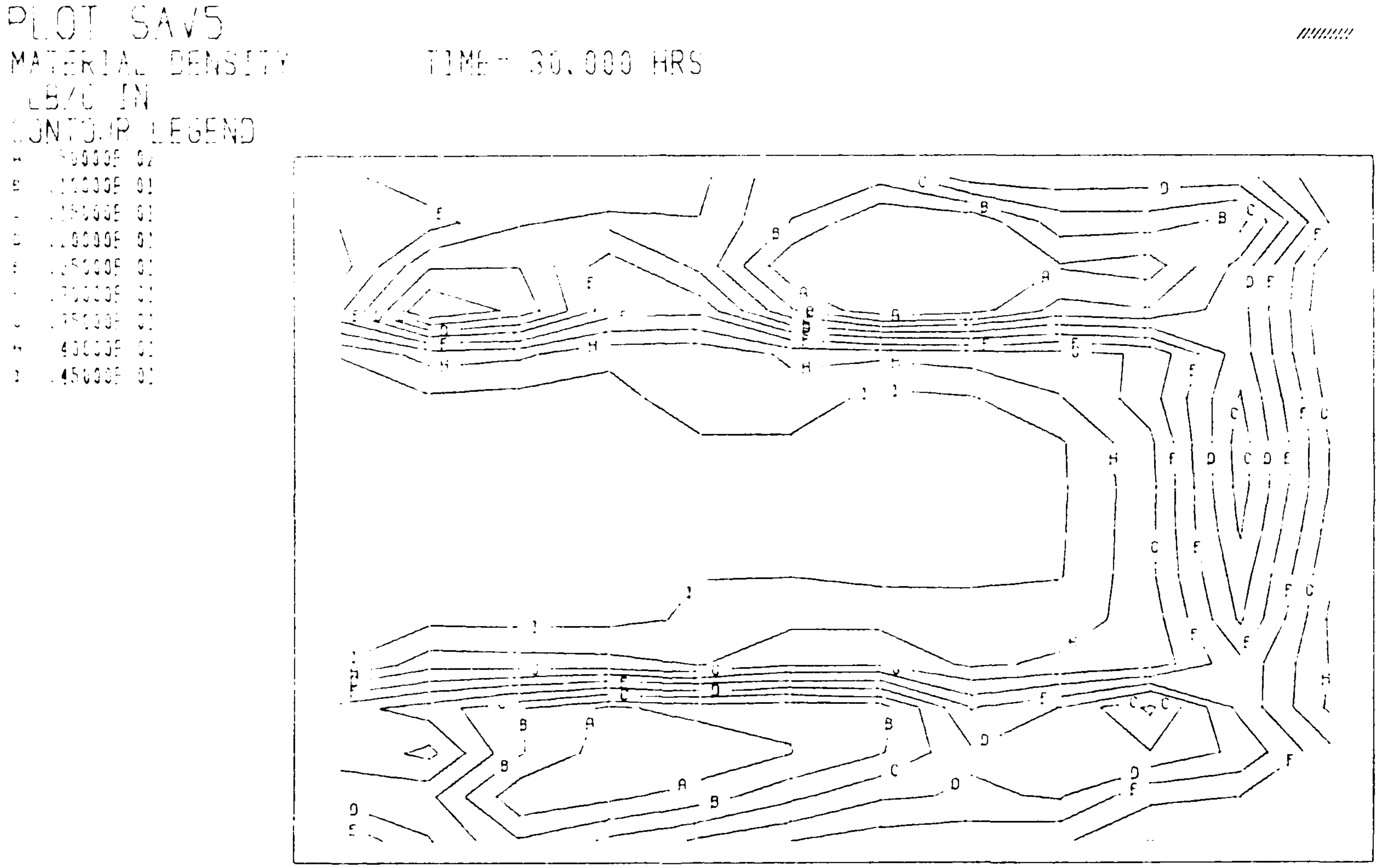


Figure 35. Material Density Contours in Carbonization Analysis.

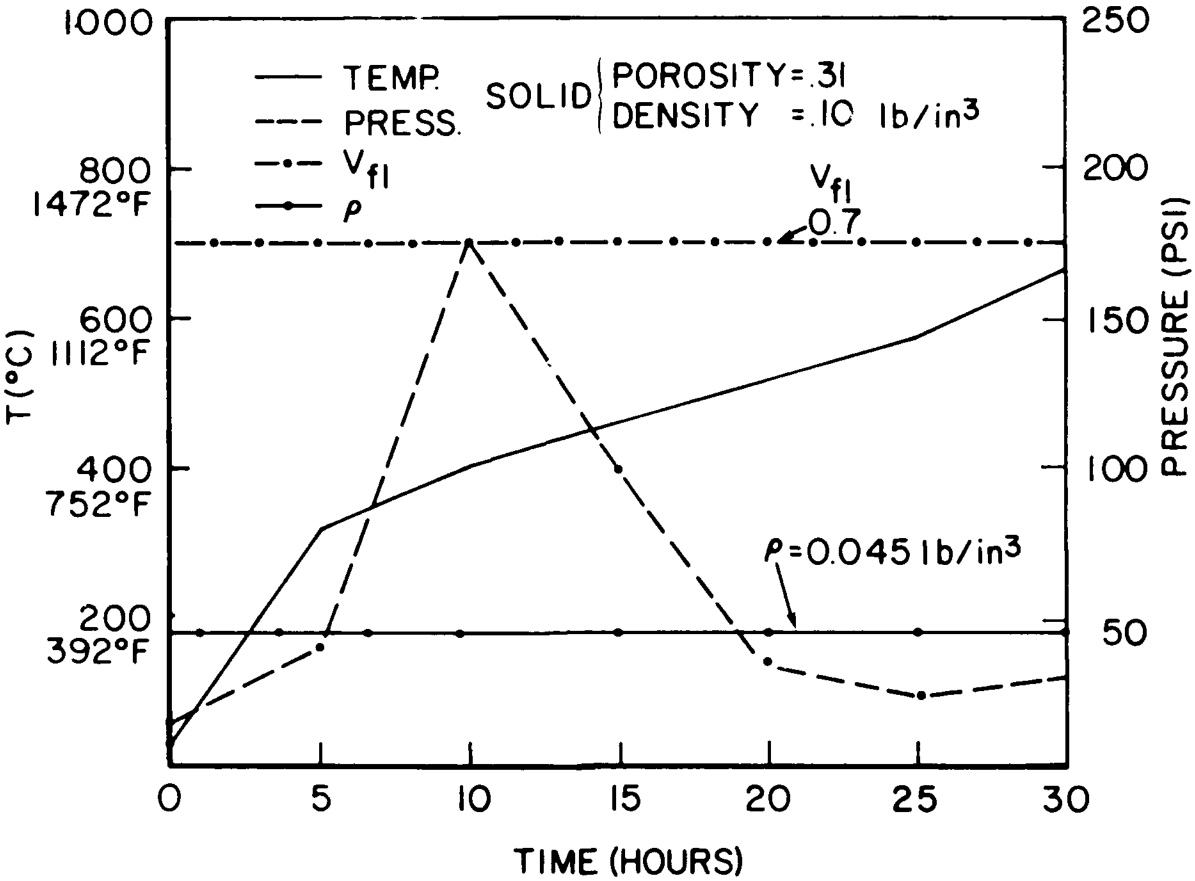


Figure 36. Variation of Response Parameters with Time at (4", 6").

CARBONIZATION ANALYSIS OUTPUT

PREFORM POROSITY = 0.55

PREFORM DENSITY = 0.065

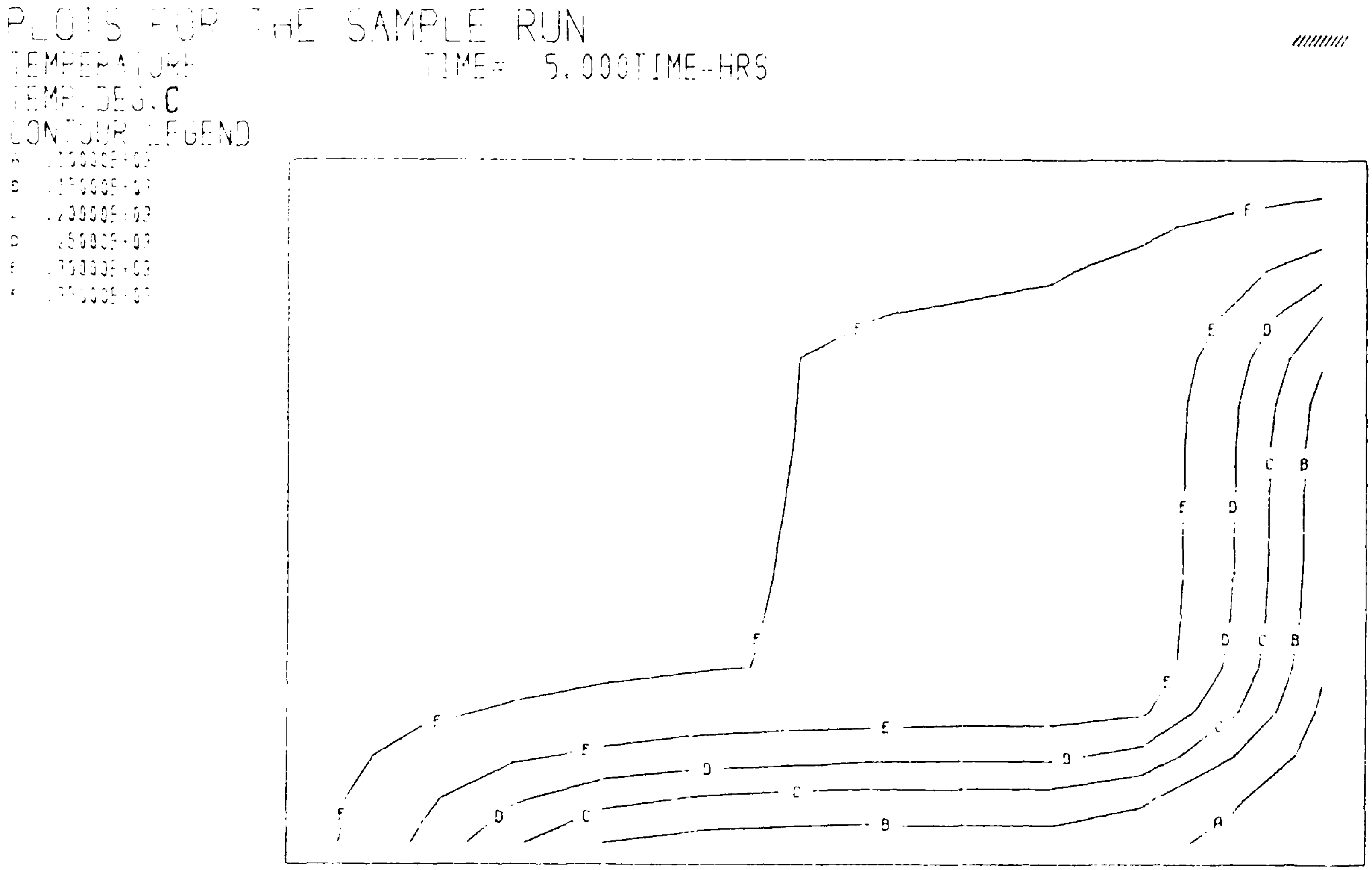


Figure 37. Temperature Contours in Carbonization Analysis.

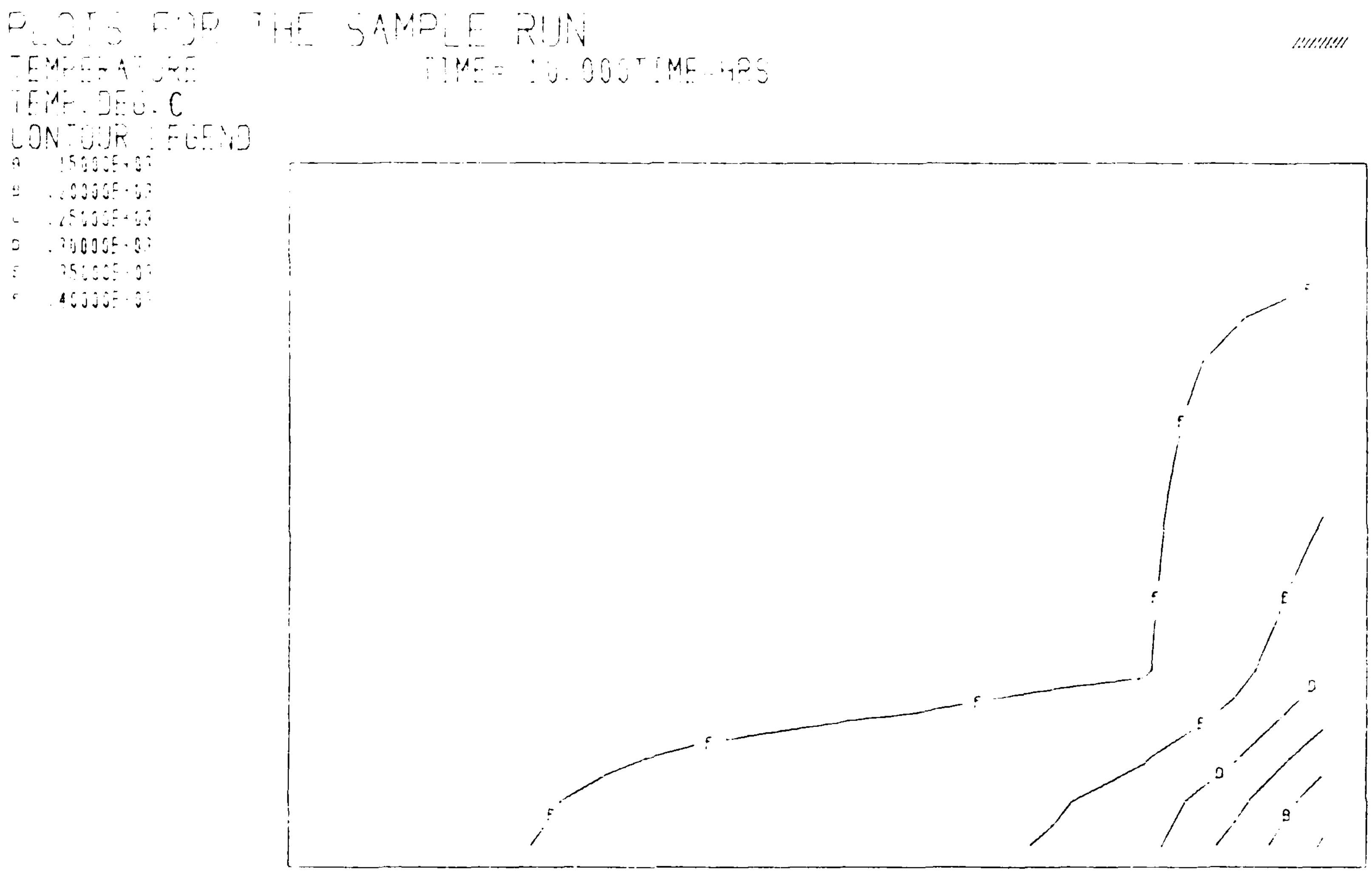


Figure 38. Temperature Contours in Carbonization Analysis.

Figure 39. Temperature Contours in Carbonization Analysis.

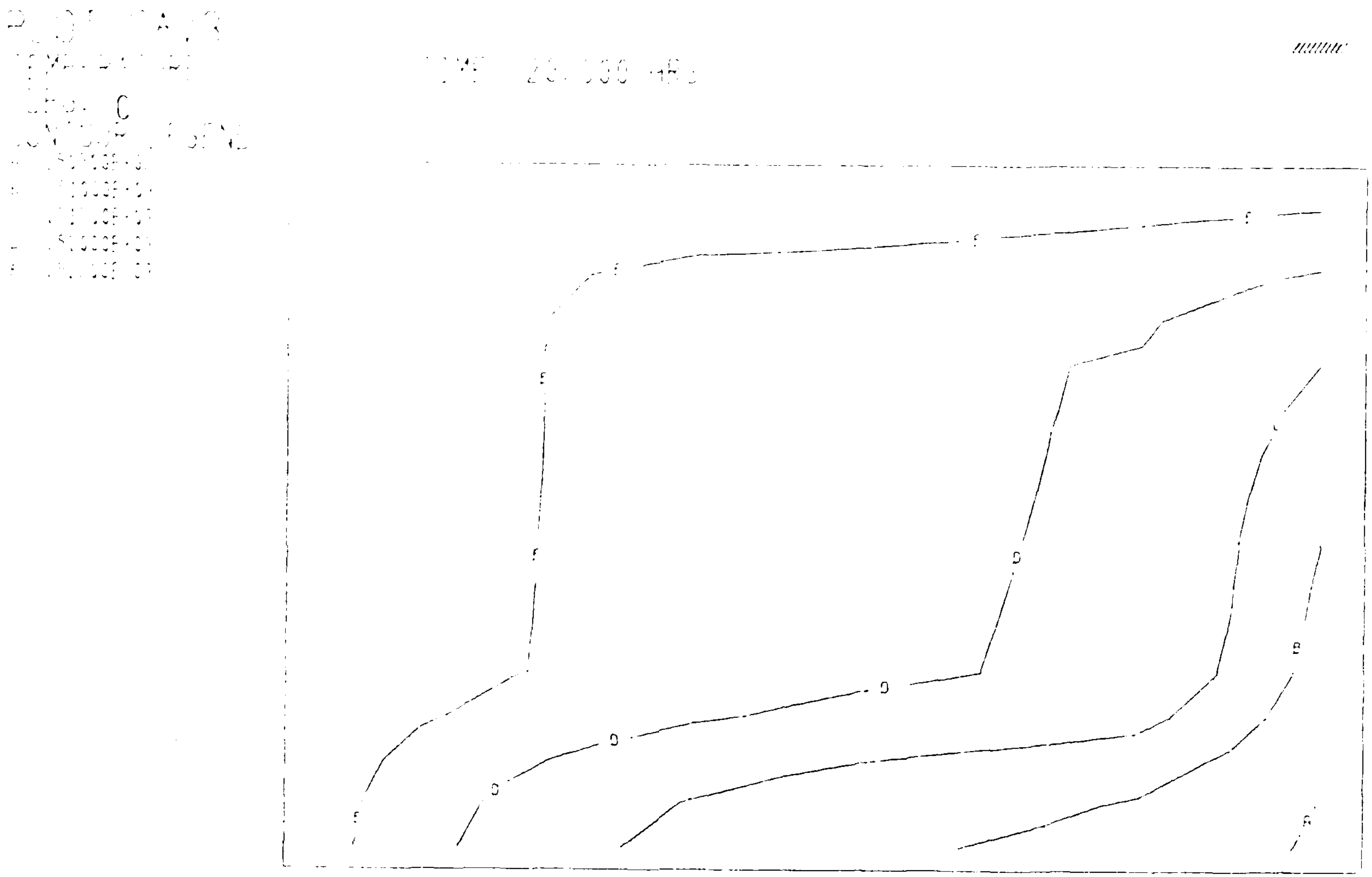


Figure 40. Temperature Contours in Carbonization Analysis.

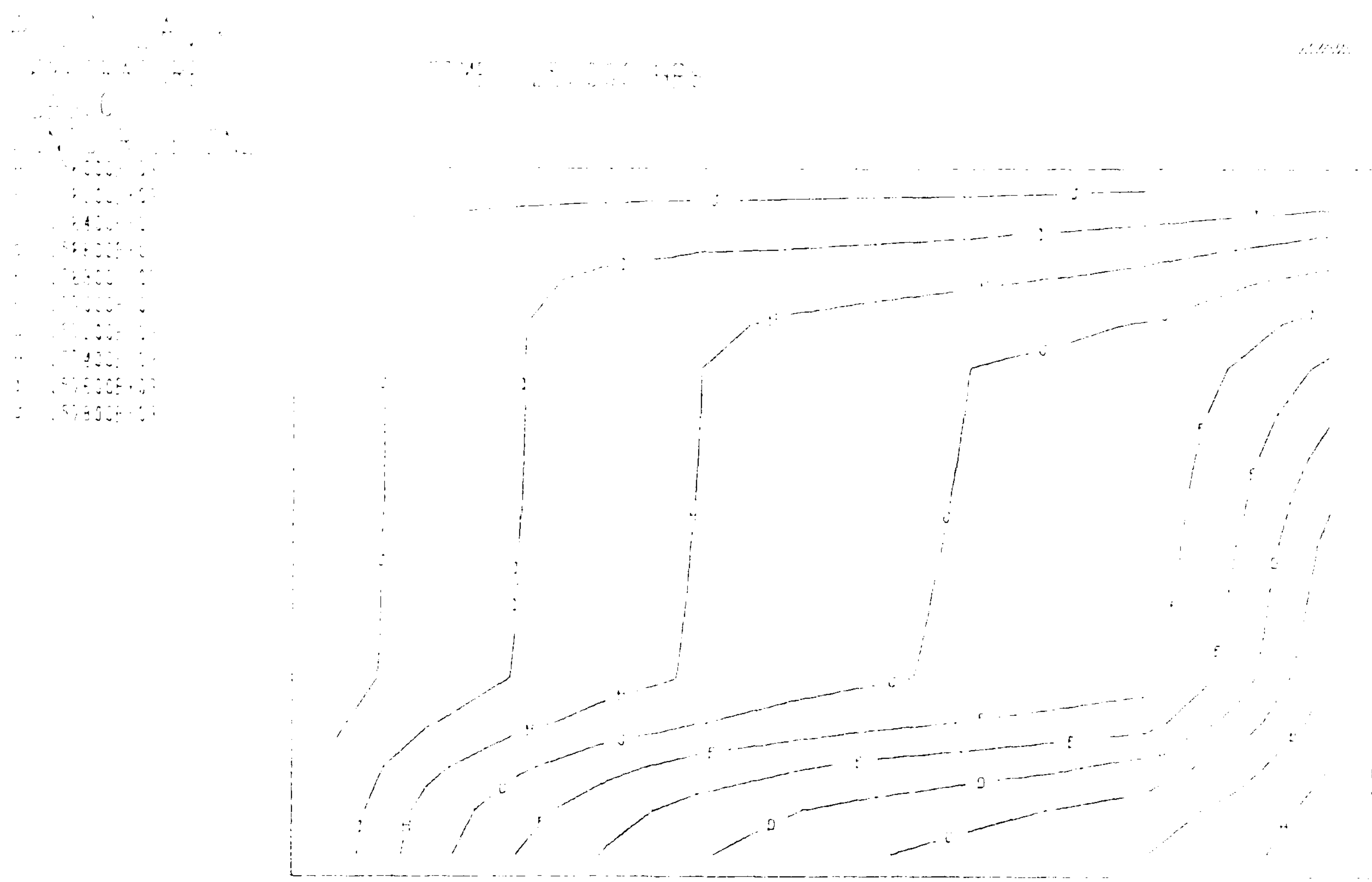


Figure 41. Temperature Contours in Carbonization Analysis.

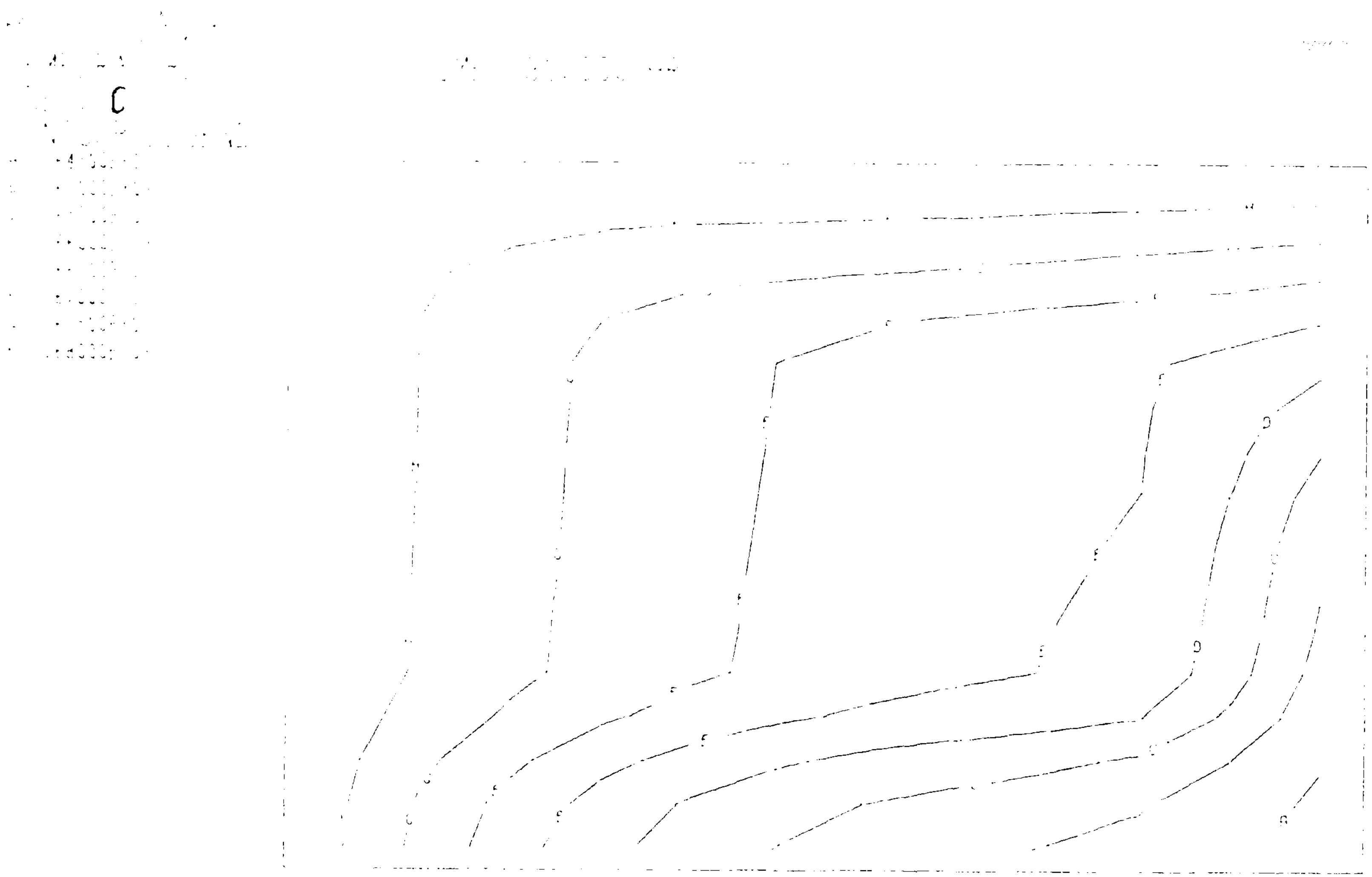
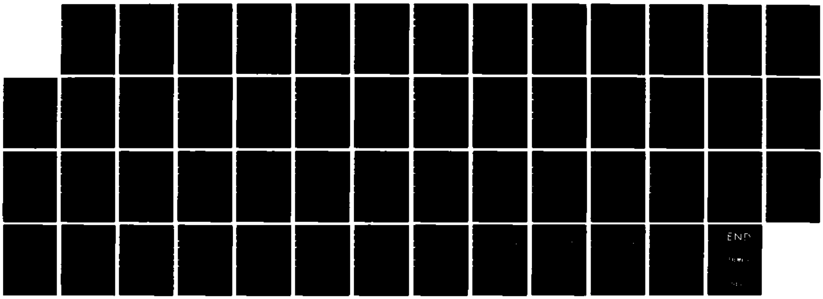
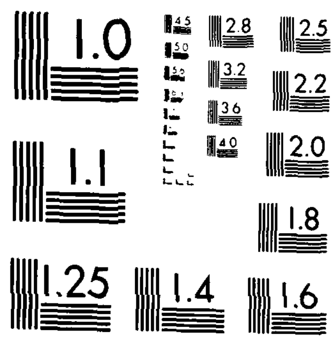


Figure 42. Temperature Contours in Carbonization Analysis.

AD-A156 889 PROCESS MODELS FOR 3D COMPOSITES(U) DAYTON UNIV OH RESEARCH INST S R SONI ET AL. MAR 85 AFWAL-TR-85-4002 F33615-81-C-5056 2/2

UNCLASSIFIED F/G 11/4 NL





MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

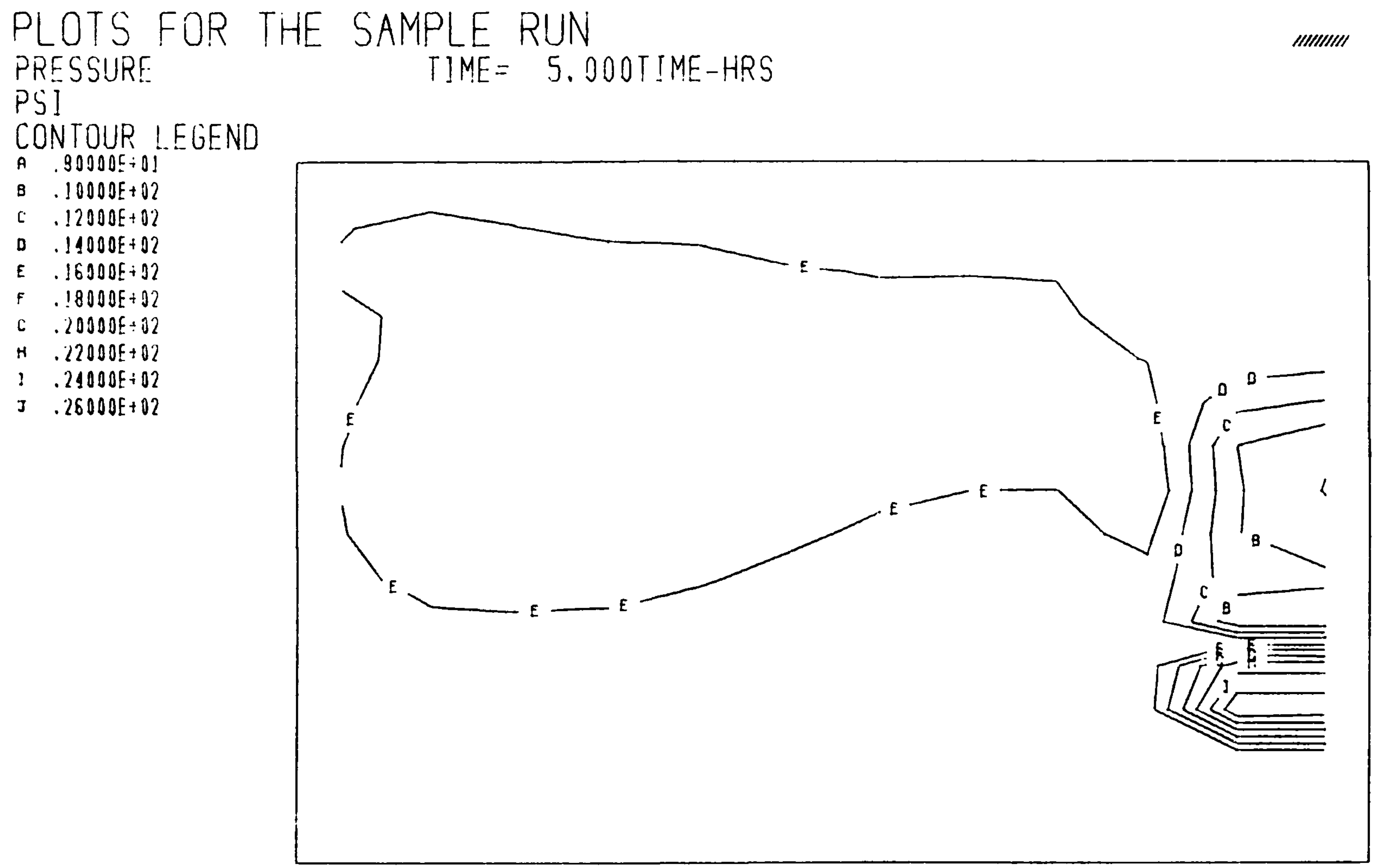


Figure 43. Pressure Contours in Carbonization Analysis.

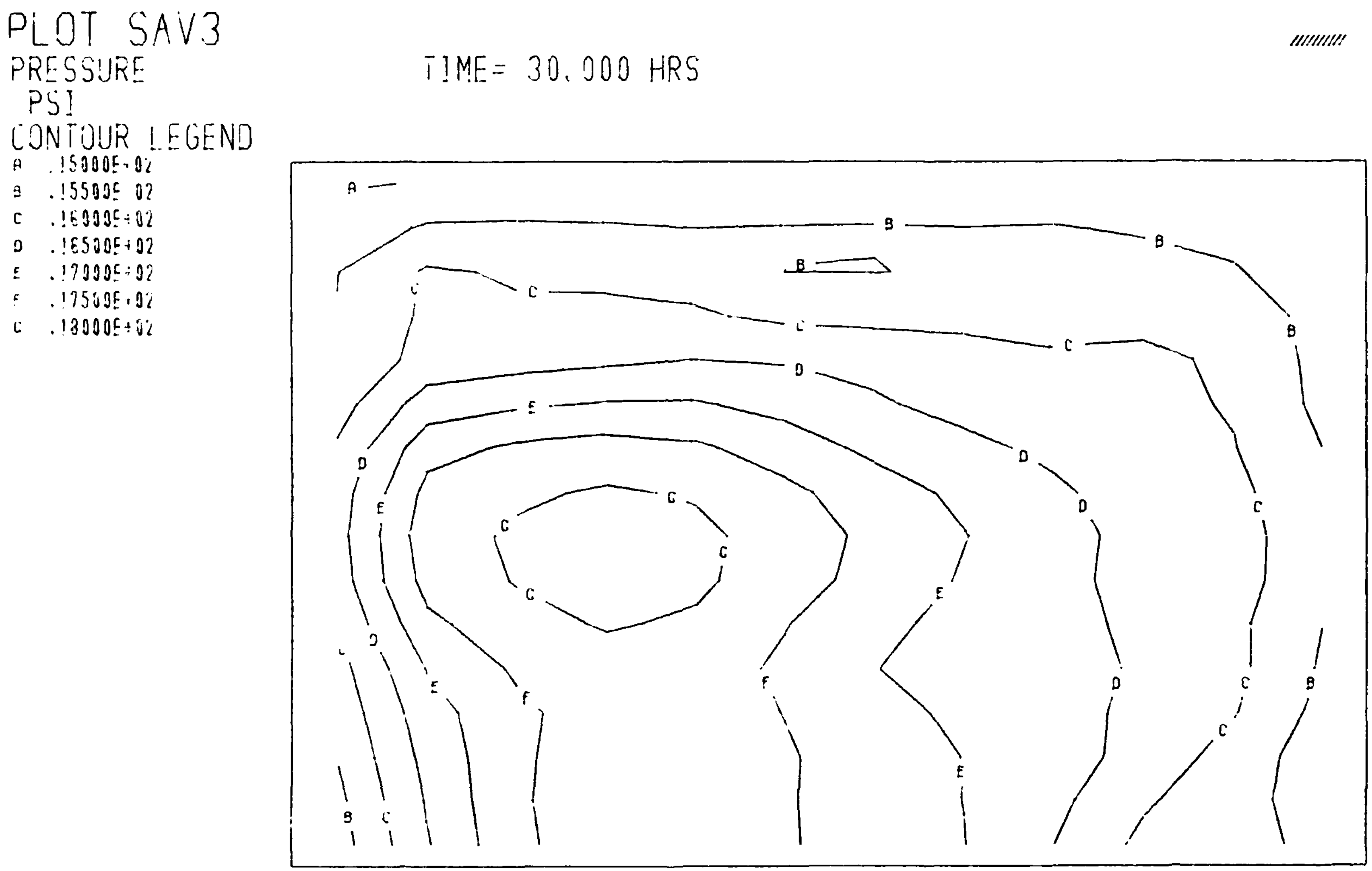


Figure 44. Pressure Contours in Carbonization Analysis.

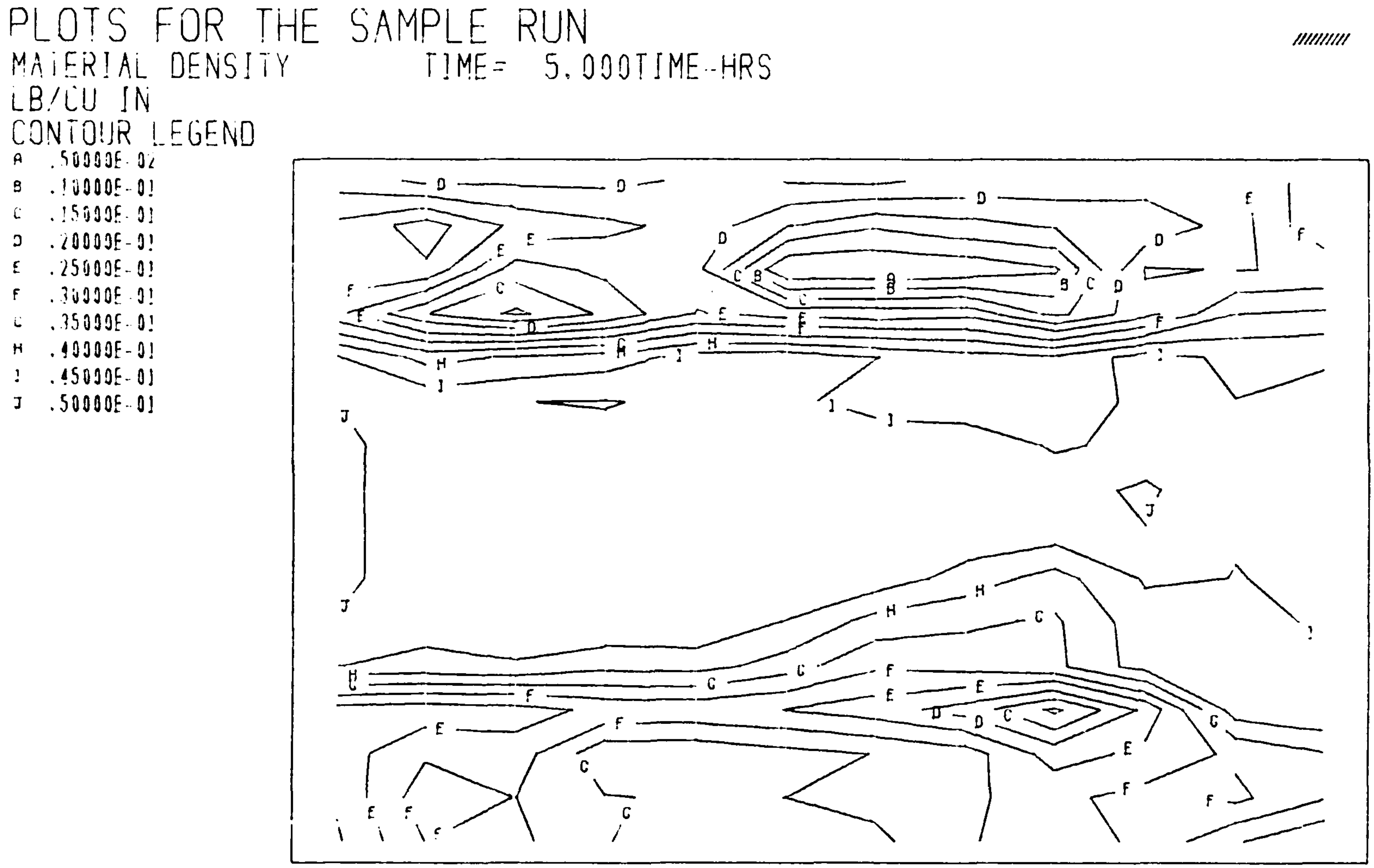


Figure 45. Material Density Contours in Carbonization Analysis.

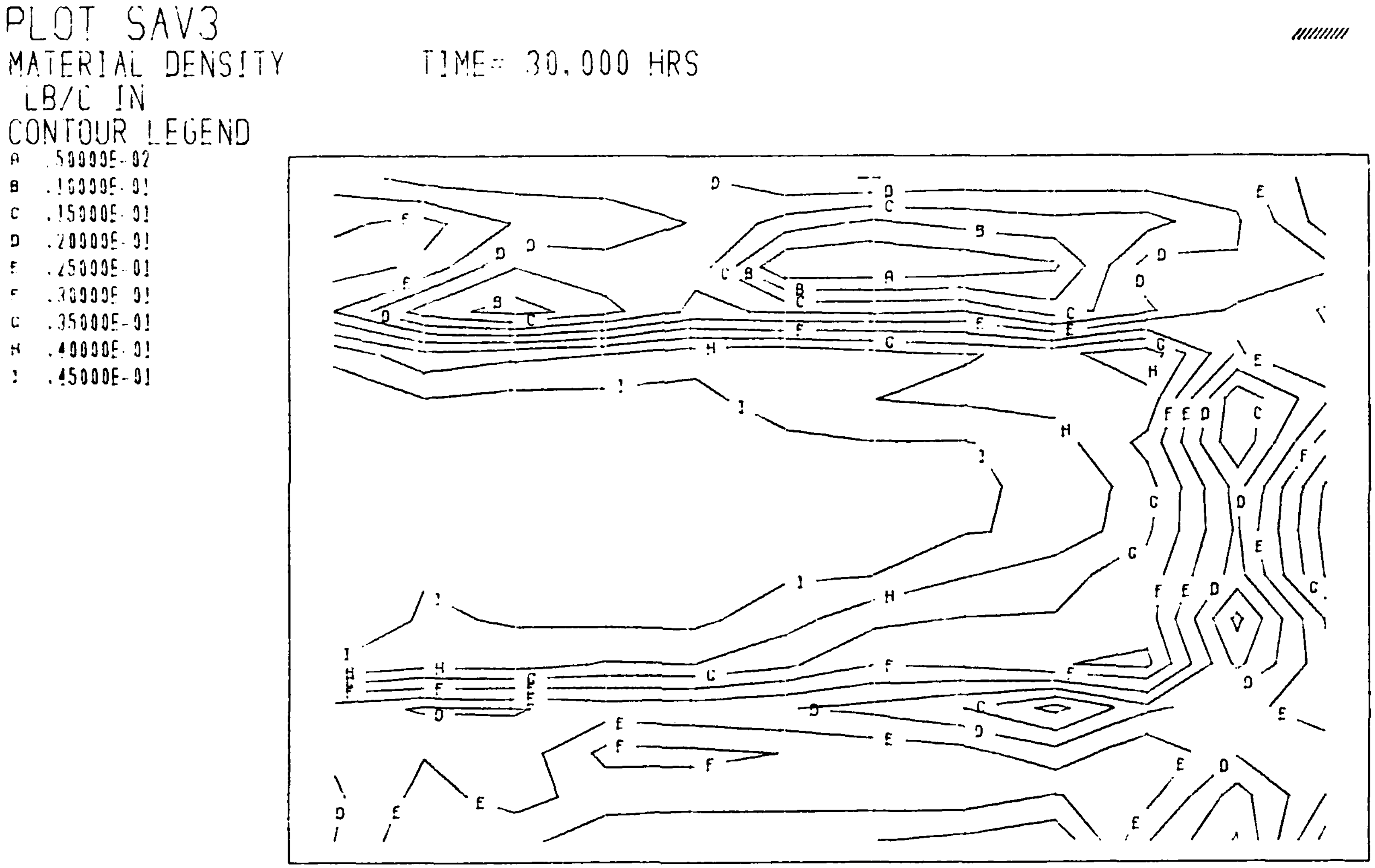


Figure 46. Material Density Contours in Carbonization Analysis.

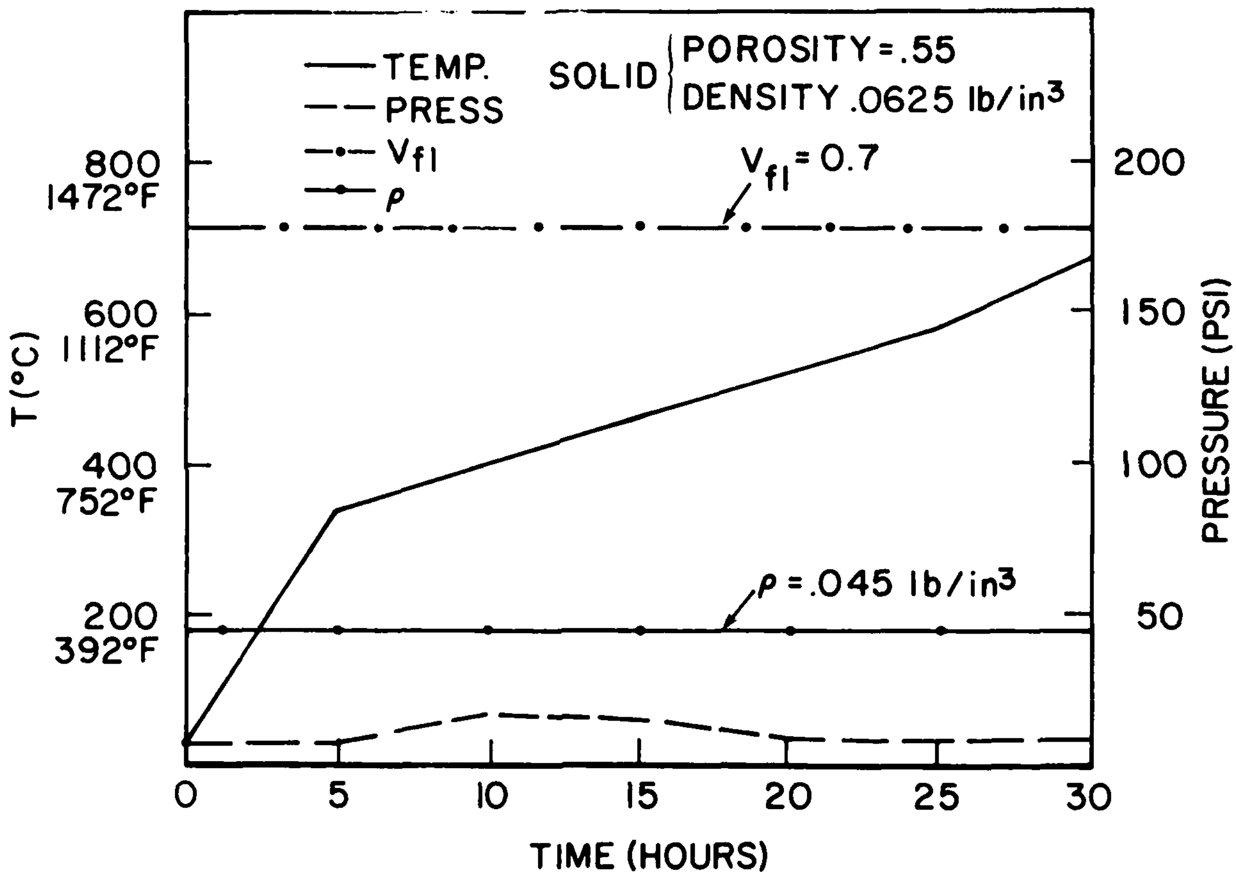


Figure 47. Variation of Response Parameters with Time at the Center of the Modeled Billet i.e. Coordinates (4", 6").

CARBONIZATION ANALYSIS OUTPUT

PREFORM POROSITY = 0.7

PREFORM DENSITY = 0.04

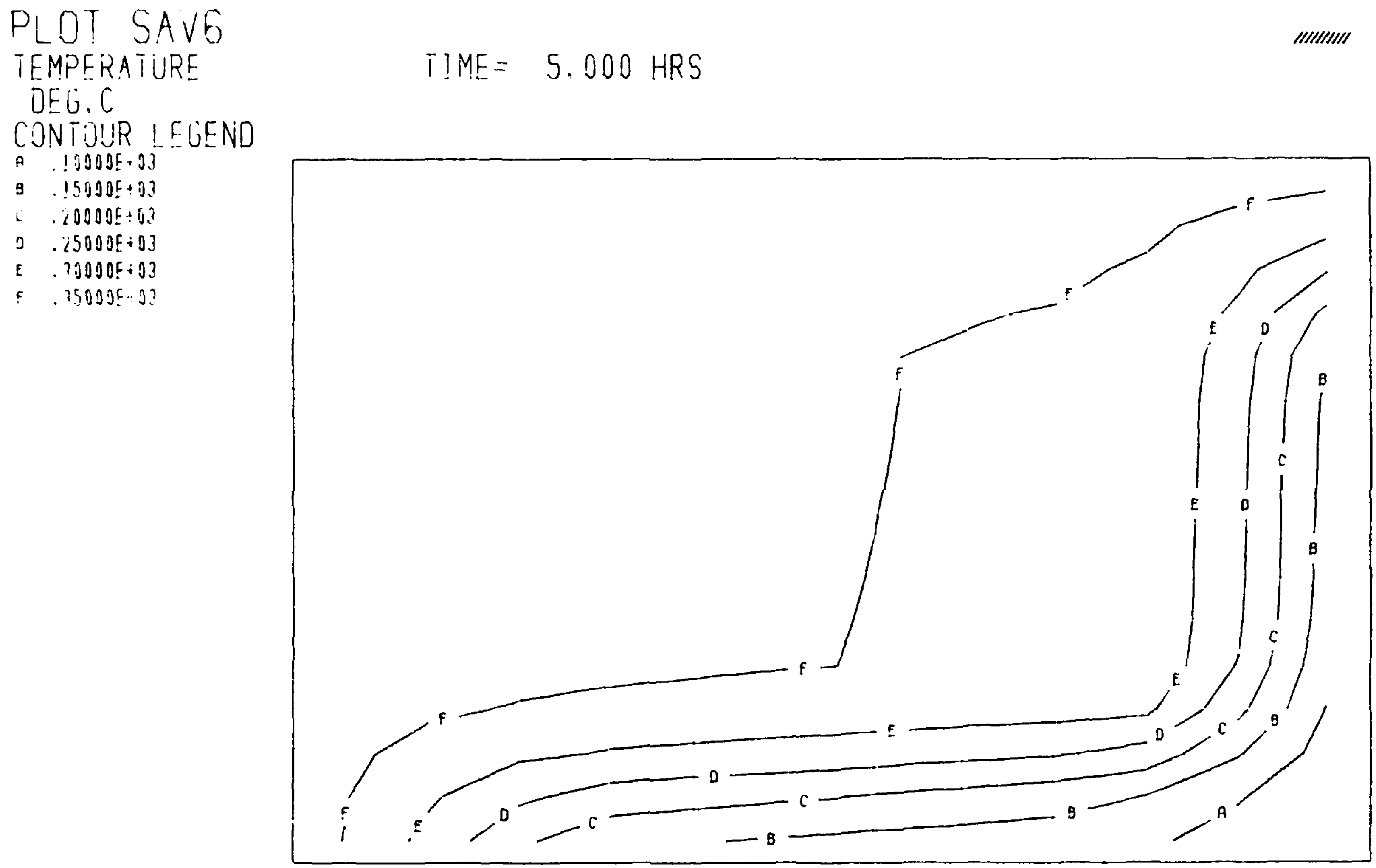


Figure 48. Temperature Contours in Carbonization Analysis.

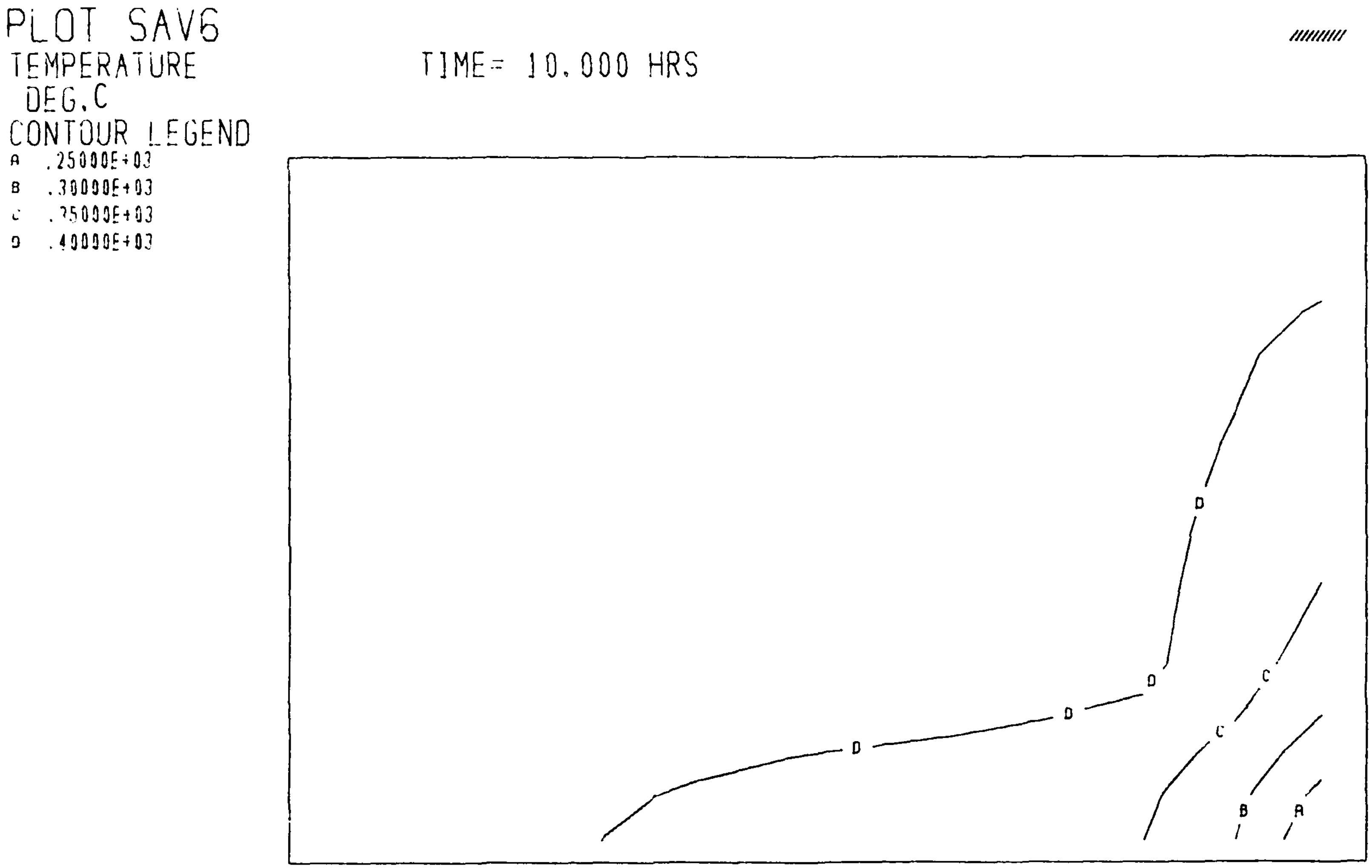


Figure 49. Temperature Contours in Carbonization Analysis.

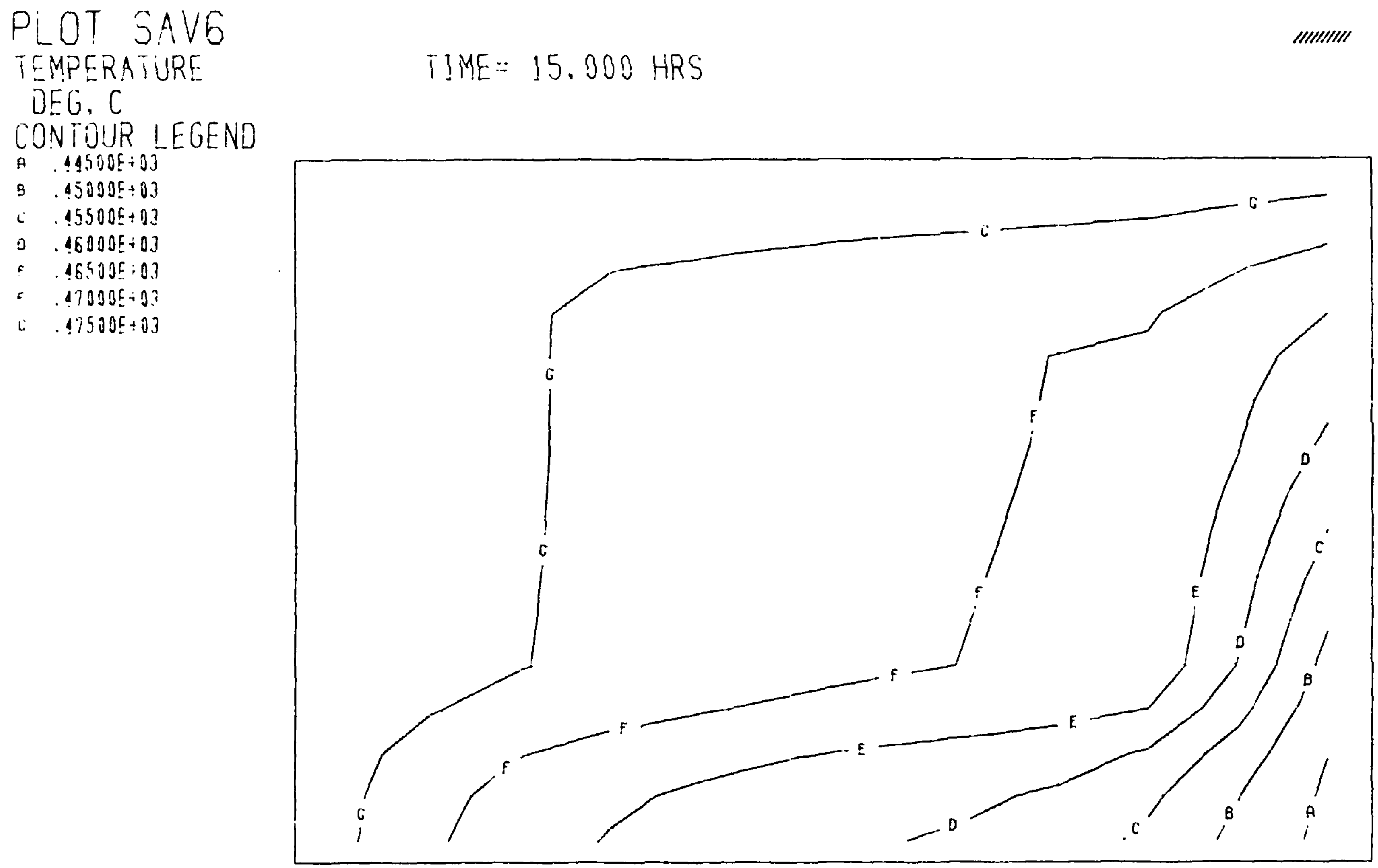


Figure 50. Temperature Contours in Carbonization Analysis.

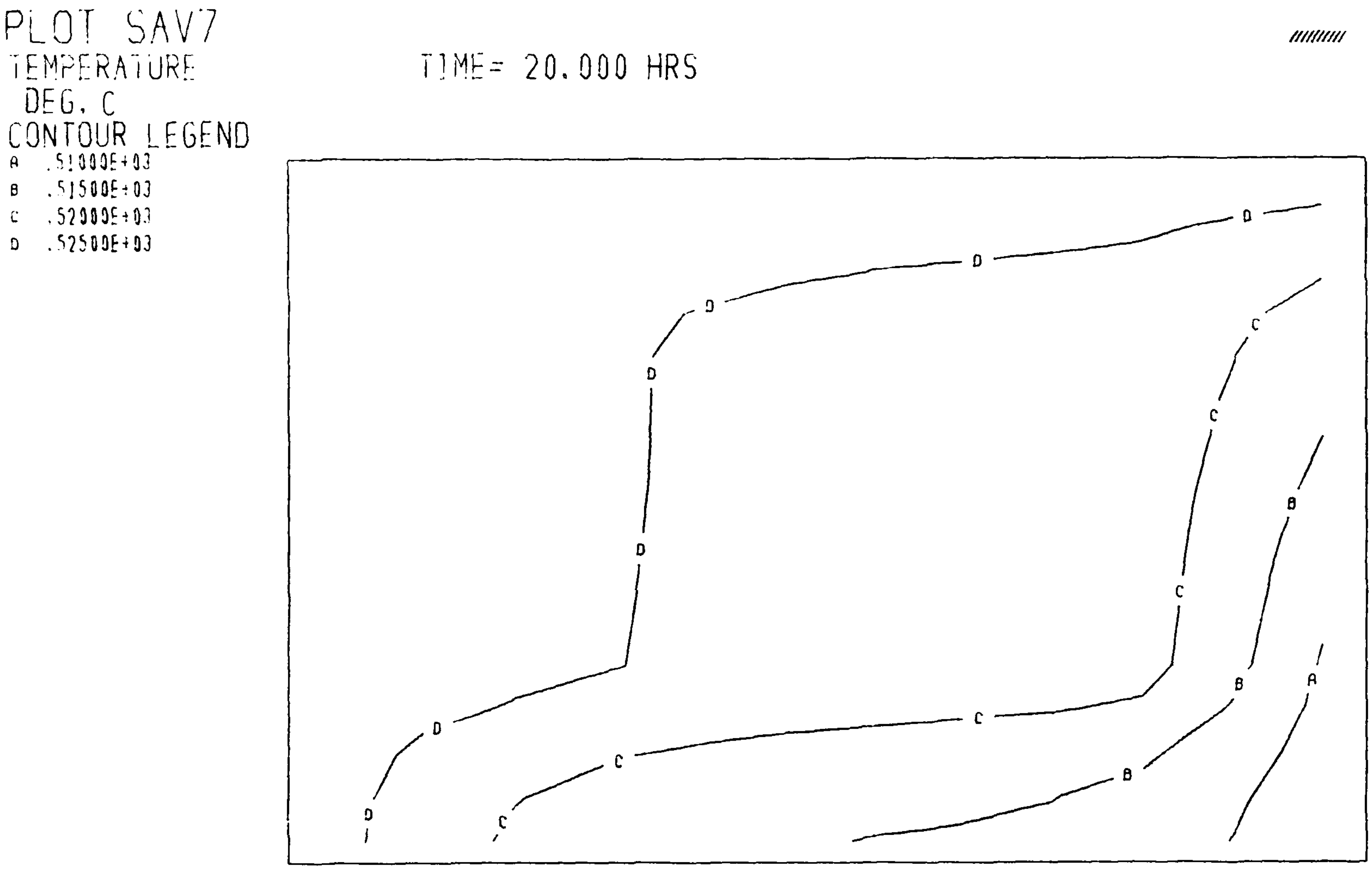


Figure 51. Temperature Contours in Carbonization Analysis.

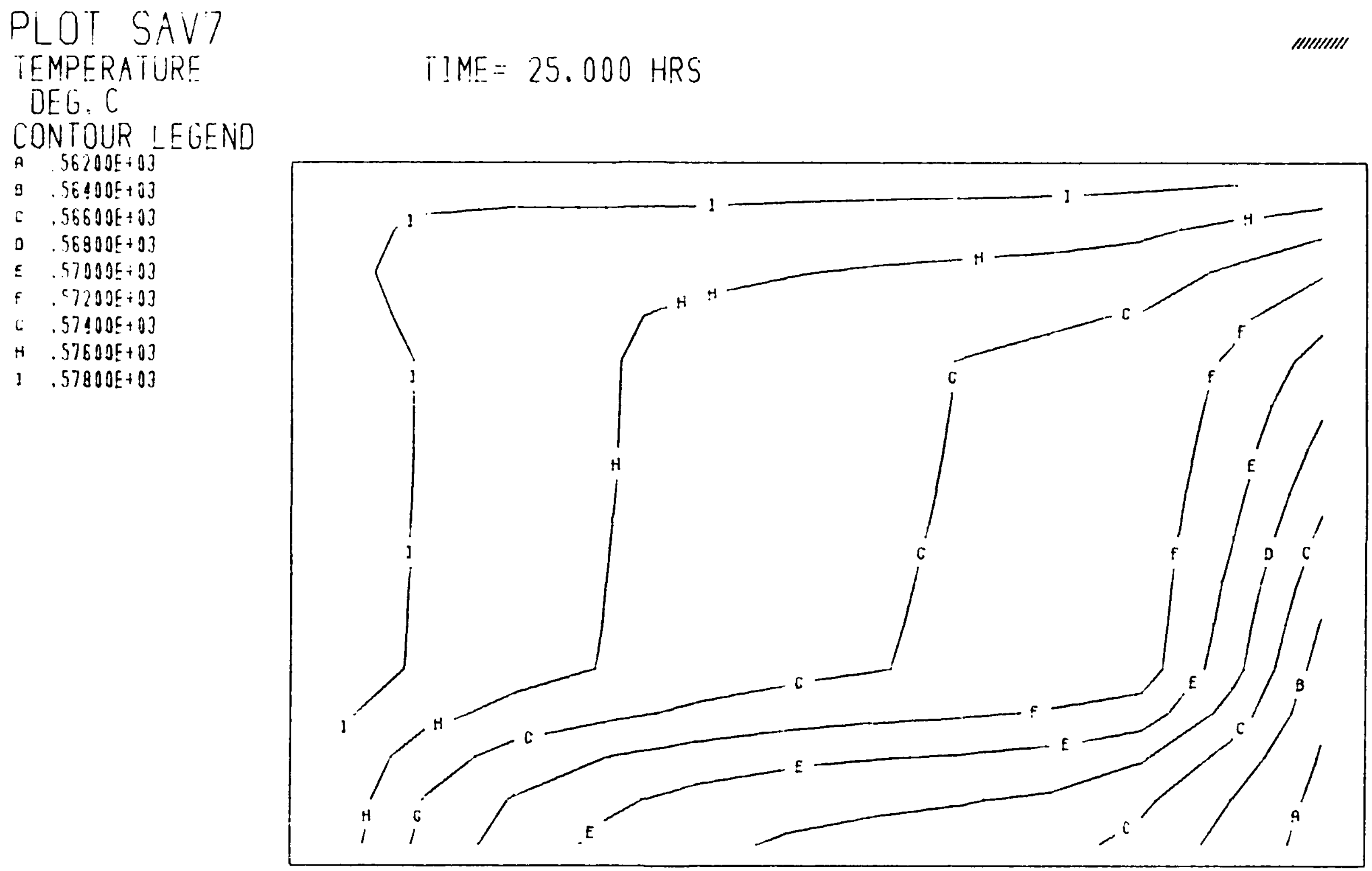


Figure 52. Temperature Contours in Carbonization Analysis.

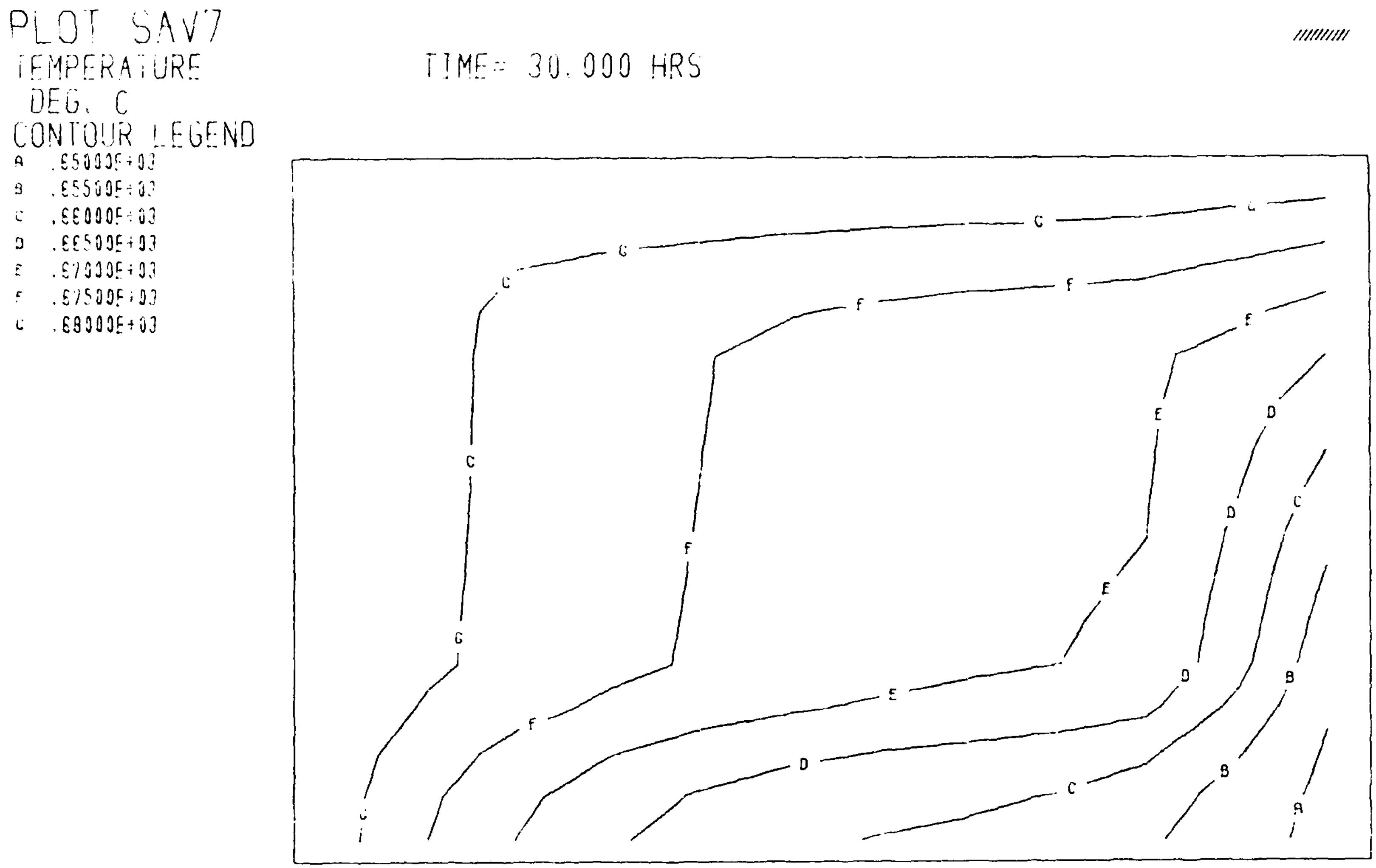


Figure 53. Temperature Contours in Carbonization Analysis.

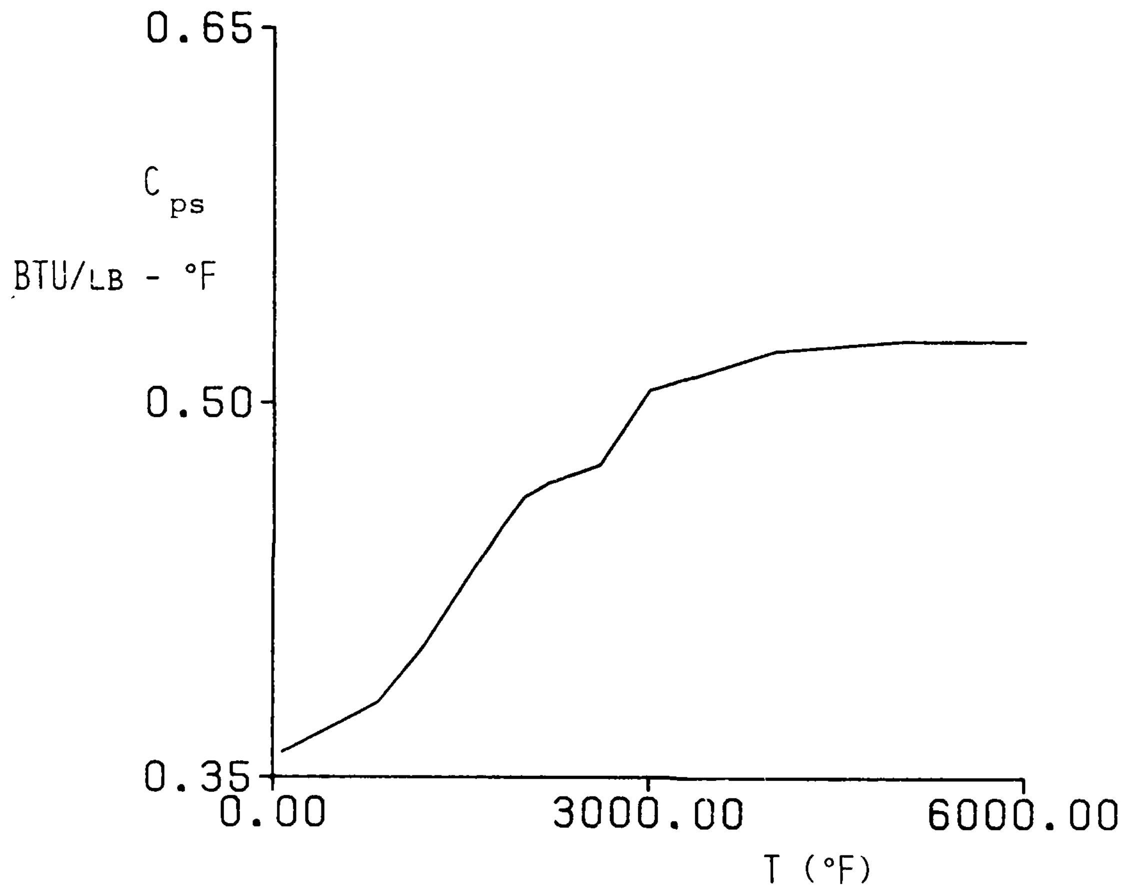


Figure 63. Solid/Filler Specific Heat C_{ps} Versus Temperature T.

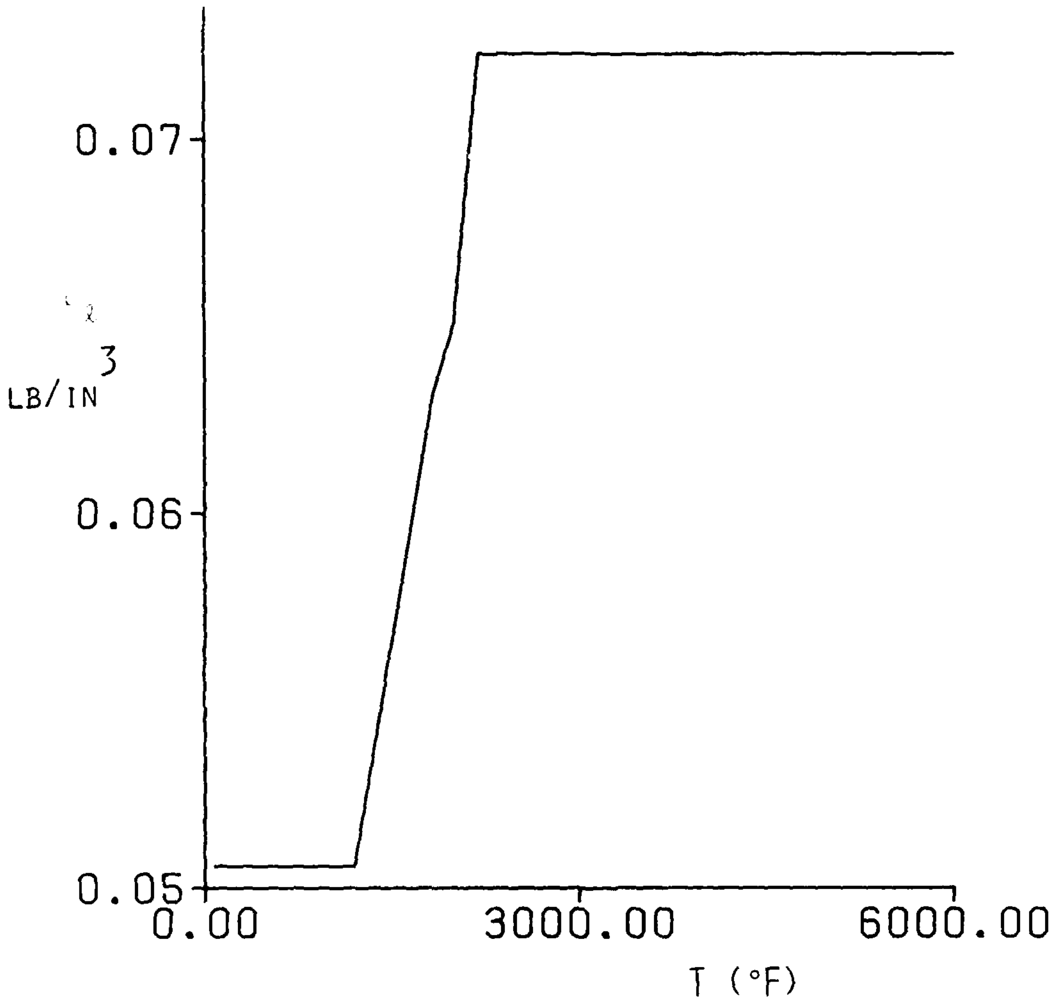


Figure 62. Liquid Pitch Density ρ_ℓ Versus Temperature T.

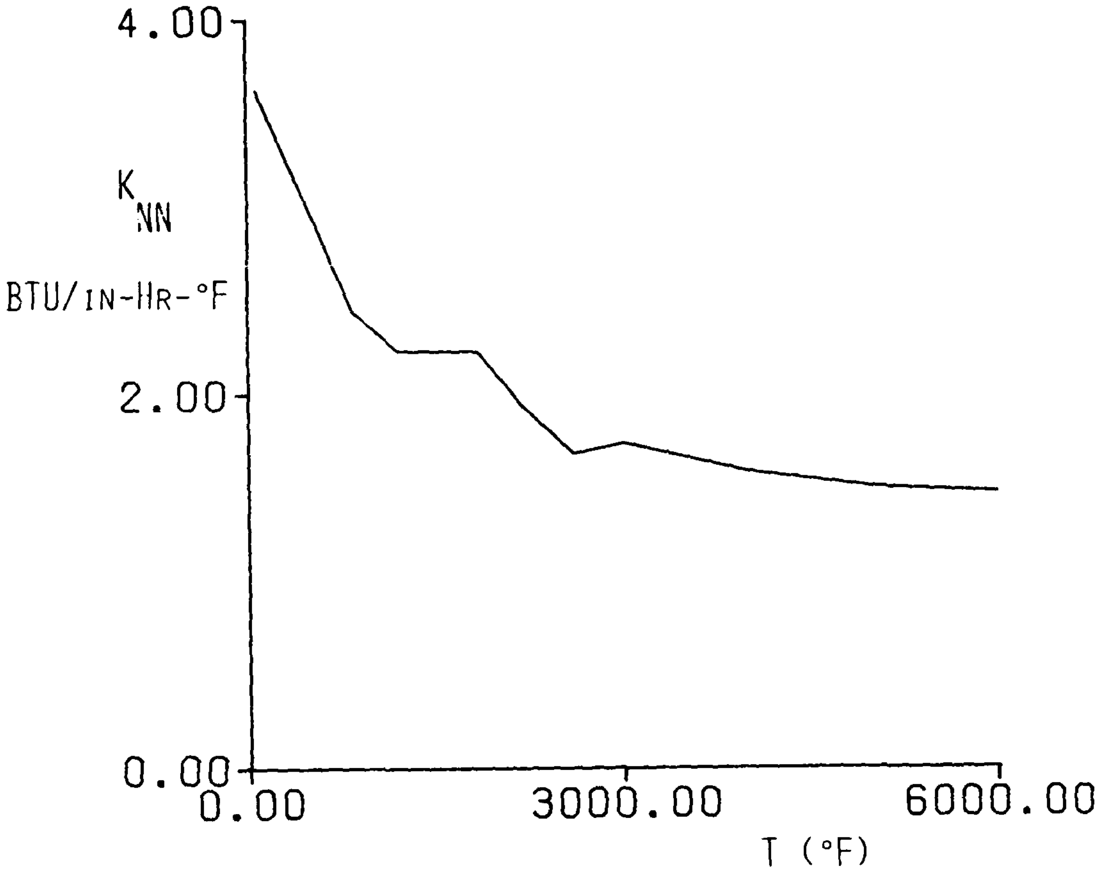


Figure 61. Solid Thermal Conductivity K_{NN} Versus Temperature T.

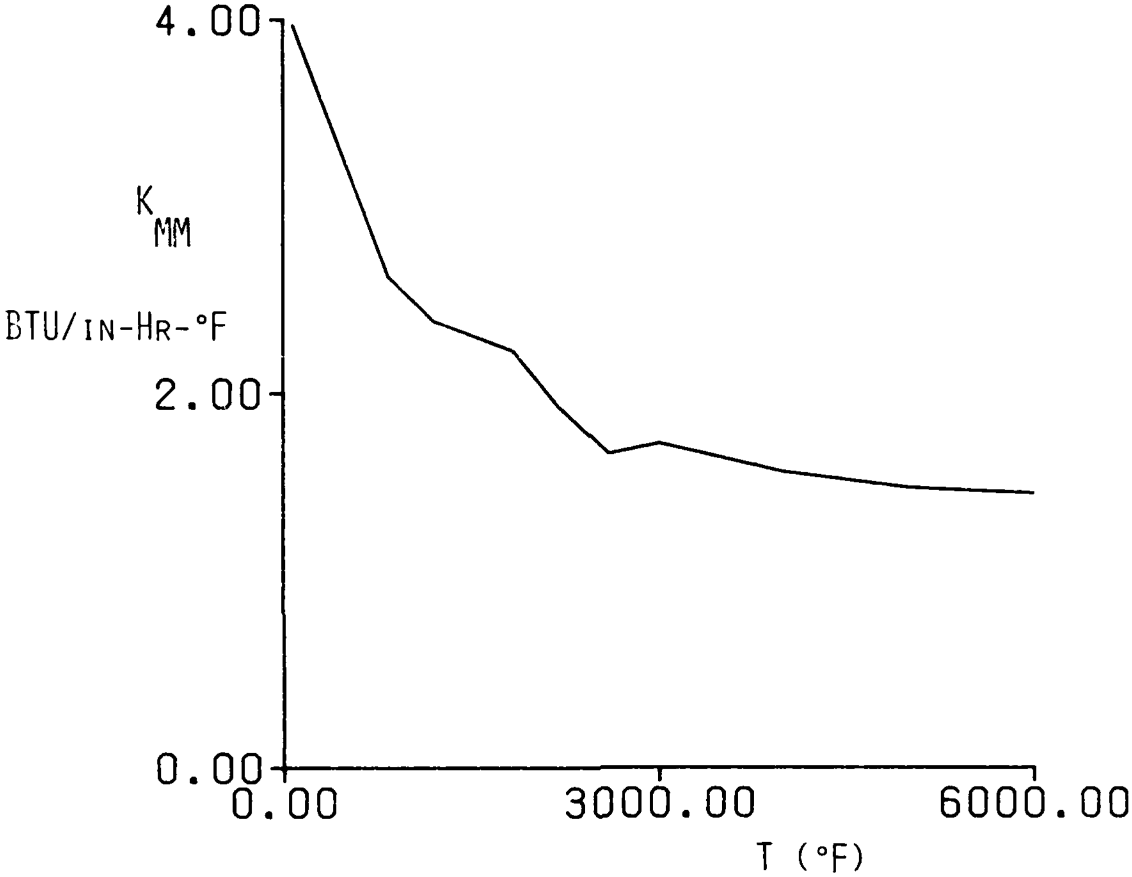


Figure 60. Solid Thermal Conductivity K_{MM} Versus Temperature T.

TABLE 9

CARBONIZED SOLID MATERIAL PROPERTY TABLE CORRESPONDING TO THE INPUT DATA QUANTITIES GIVEN ON PAGE 21, i.e.

T, K_{MM}, K_{NN}, M_g, $\frac{\partial \rho_\ell}{\partial T}$	Format (4F10.0, 10X, F10.0)
C_{ps}	Format (30X, F10.0)
C_{pg}, $C_{p\ell}$	Format (30X, 2F10.0)

at each temperature T is:

537.	3.9688	3.6242	16.		0.05058
			0.360		
			0.500	0.82	
1302.	2.6231	2.4380	16.		0.05058
			0.380		
			0.500	0.82	
1562.	2.3868	2.228	16.		0.05058
			0.402		
			0.500	0.82	
2292.	2.2261	2.2256	16.		0.06322
			0.451		
			0.490	0.82	
2460.	2.0937	2.0936	16.		0.06503
			0.462		
			0.485	0.82	
2660.	1.9284	1.9283	16.		0.07226
			0.468		
			0.468	0.82	
3060.	1.6793	1.6793	16.		0.07226
			0.475		
			0.475	0.82	
3460.	1.734	1.734	16.		0.07226
			0.505		
			0.505	0.82	
4460.	1.578	1.578	16.		0.07226
			0.521		
			0.521	0.82	
5460.	1.494	1.494	16.		0.07226
			0.525		
			0.525	0.82	
6460.	1.464	1.464	16.		0.07226
			0.525		
			0.525	0.82	

In the following Figures the temperature-dependent parameters from the foregoing table are given. Graphitization temperature variation with time is also given. Similar plots could be obtained for carbonized liquid material, since in the case considered here, the difference between the material properties for carbonized liquid and carbonized solid is small, material property plots are given only for carbonized solid.

TABLE 8

CARBONIZED LIQUID MATERIAL PROPERTY TABLE CORRESPONDING TO THE INPUT DATA QUANTITIES GIVEN ON PAGE 21, i.e.

T, K_{MM}, K_{NN}, M_g, $\frac{\partial \rho_\ell}{\partial T}$	Format (4F10.0, 10X, F10.0)
C_{ps}	Format (30X, F10.0)
C_{pg}, $C_{p\ell}$	Format (30X, 2F10.0)

For each value of T are:

537.	3.795	3.711	16.		0.05058
			0.360		
			0.500	0.82	
1302.	2.507	2.458	16.		0.05058
			0.380		
			0.500	0.82	
1662.	2.281	2.238	16.		0.05058
			0.402		
			0.500	0.82	
2292.	2.212	2.211	16.		0.06322
			0.451		
			0.490	0.82	
2460.	2.0852	2.0850	16.		0.06503
			0.462		
			0.485	0.82	
2660.	1.9245	1.9245	16.		0.07226
			0.468		
			0.468	0.82	
3060.	1.6791	1.6791	16.		0.07226
			0.475		
			0.475	0.82	
3460.	1.734	1.734	16.		0.07226
			0.505		
			0.505	0.82	
4460.	1.578	1.578	16.		0.07226
			0.521		
			0.521	0.82	
5460.	1.494	1.494	16.		0.07226
			0.525		
			0.525	0.82	
6460.	1.464	1.464	16.		0.07226
			0.525		
			0.525	0.82	

Curing time table for graphitization is:
Time, Temp Format (8F10.0)

0.	537.	1.	1031.4	3.	1679.4	5.	2111.4
7.	2291.4	11.	2615.4	13.	2813.4	16.	3011.4
19.	3101.4	23.	3353.4	29.	5225.4	30.	5387.4

In these tables T is given in °R where as in plots T is given in (°F).

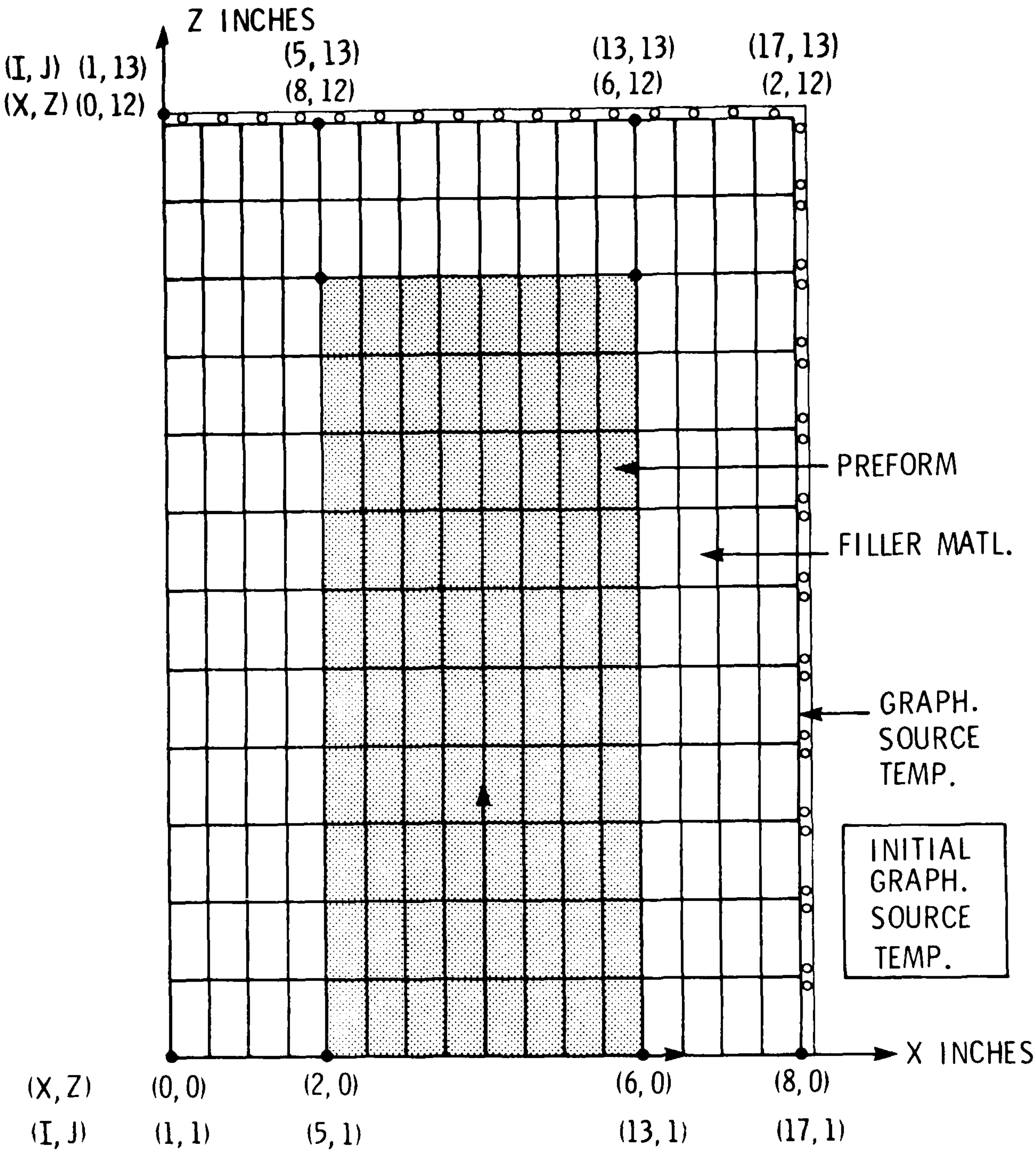


Figure 59. Finite Element Grid of Billet for Graphitization.

For graphitization analysis, the same two-billet can used for carbonization, Figure 6, has been considered. The finite element grid and the boundary conditions shown in Figure 6 have been used. The temperature dependent material properties of the billet preform and liquid pitch after carbonization are given in Tables 8 and 9. These properties do not necessarily correspond to any of the three cases of billets analyzed for carbonization process in this report. The graphitization process temperature schedule is given in Table 8 and also in Figure 65. The PEM computer input data for this problem is given in Table 10. The processing analysis is conducted up to 30 hours. Figure 66 shows the temperature profile results at two locations of the billet during graphitization.

GRAPHITIZATION ANALYSIS

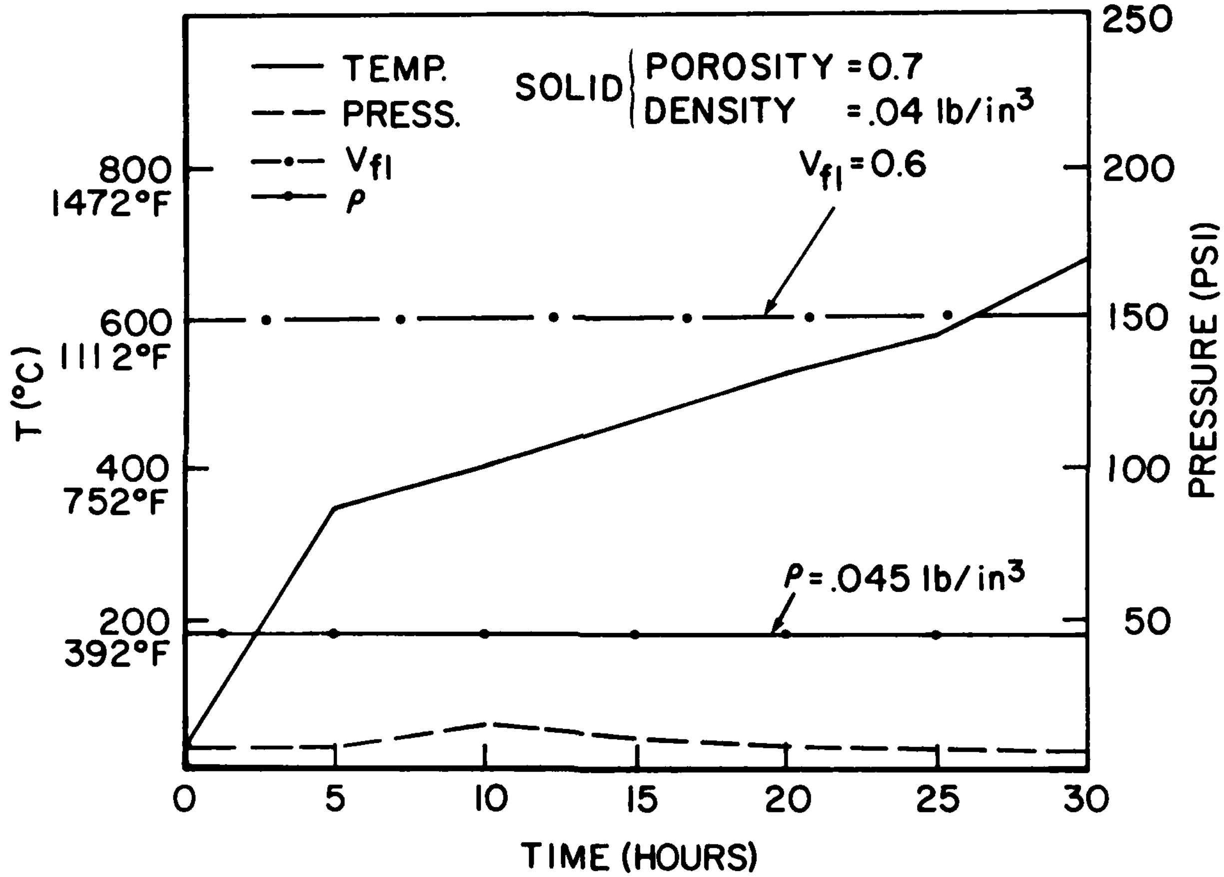


Figure 58. Variation of Response Parameters with Time at the Center of the Modeled Billet i.e. Coordinates (4", 6").

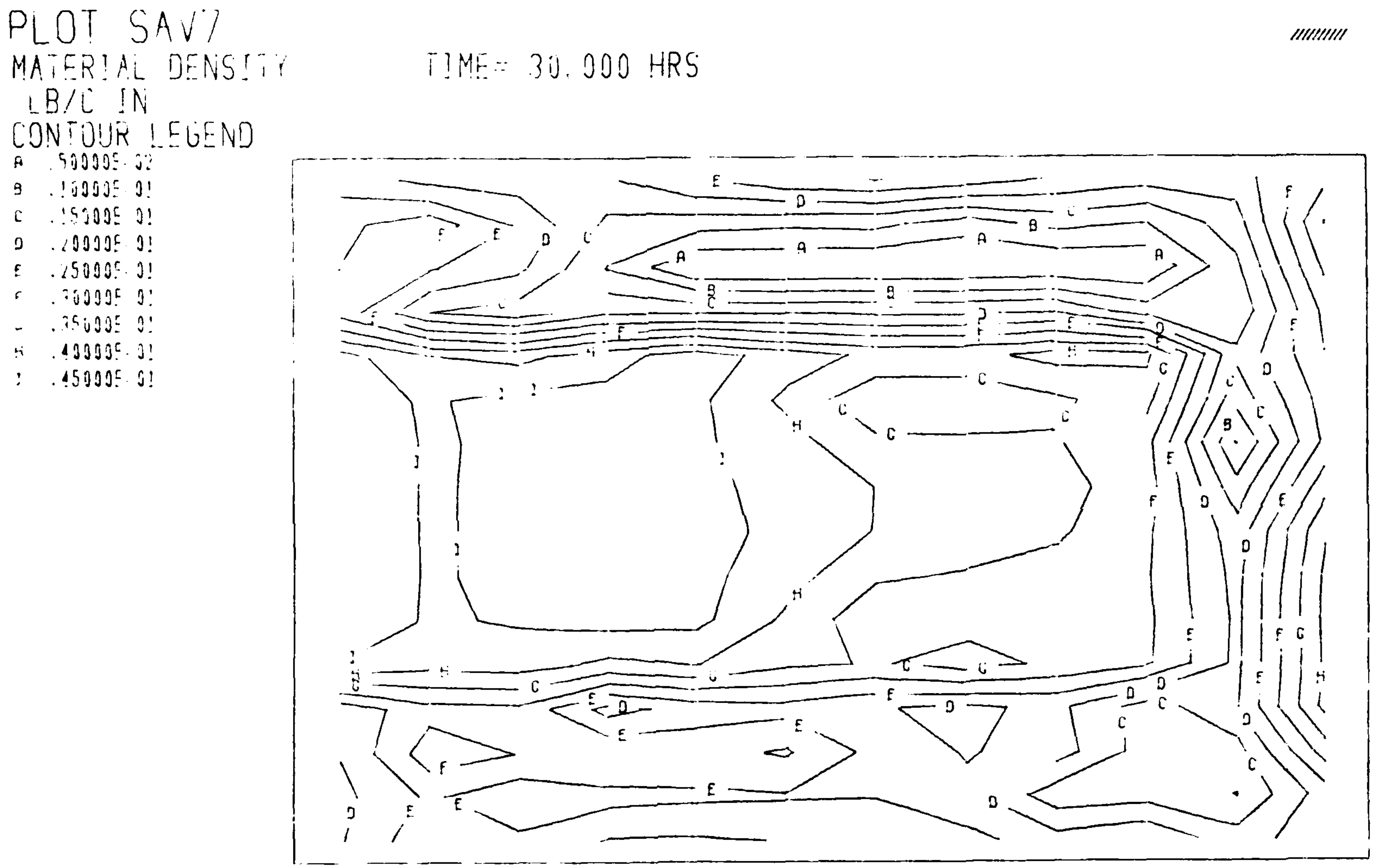


Figure 57. Material Density Contours in Carbonization Analysis.

Figure 56. Material Density Contours in Carbonization Analysis.

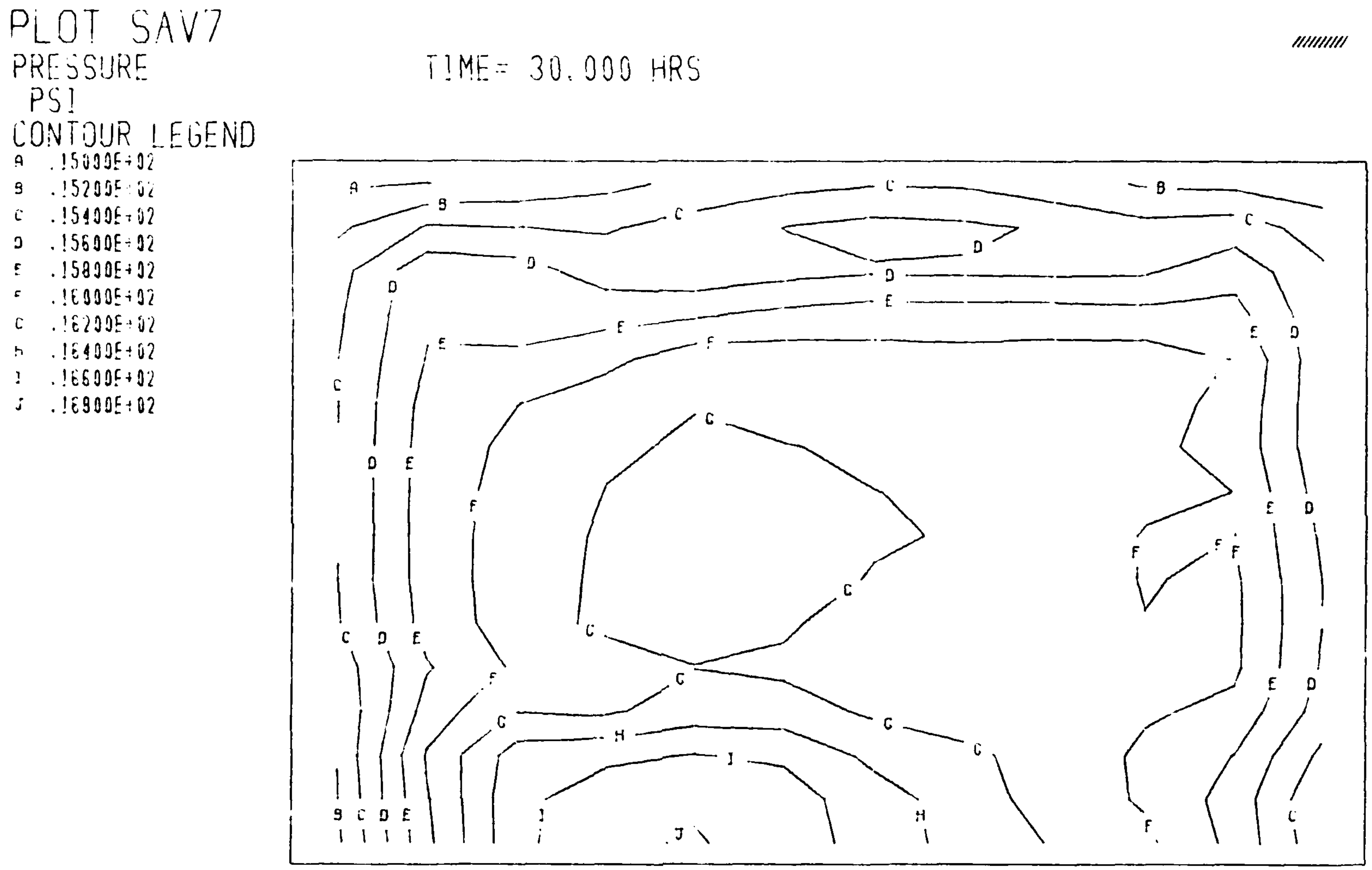


Figure 55. Pressure Contours in Carbonization Analysis.

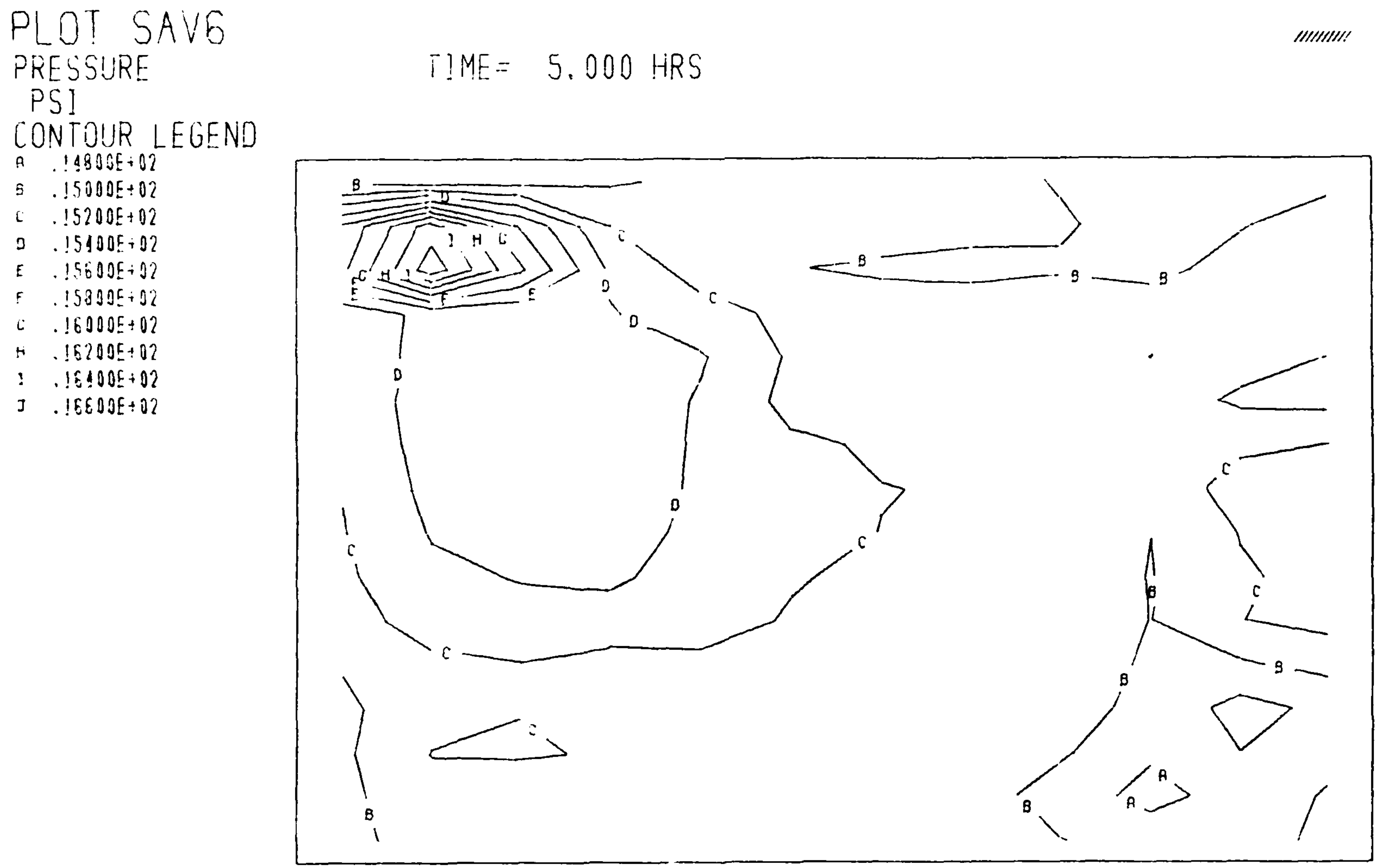


Figure 54. Pressure Contours in Carbonization Analysis.

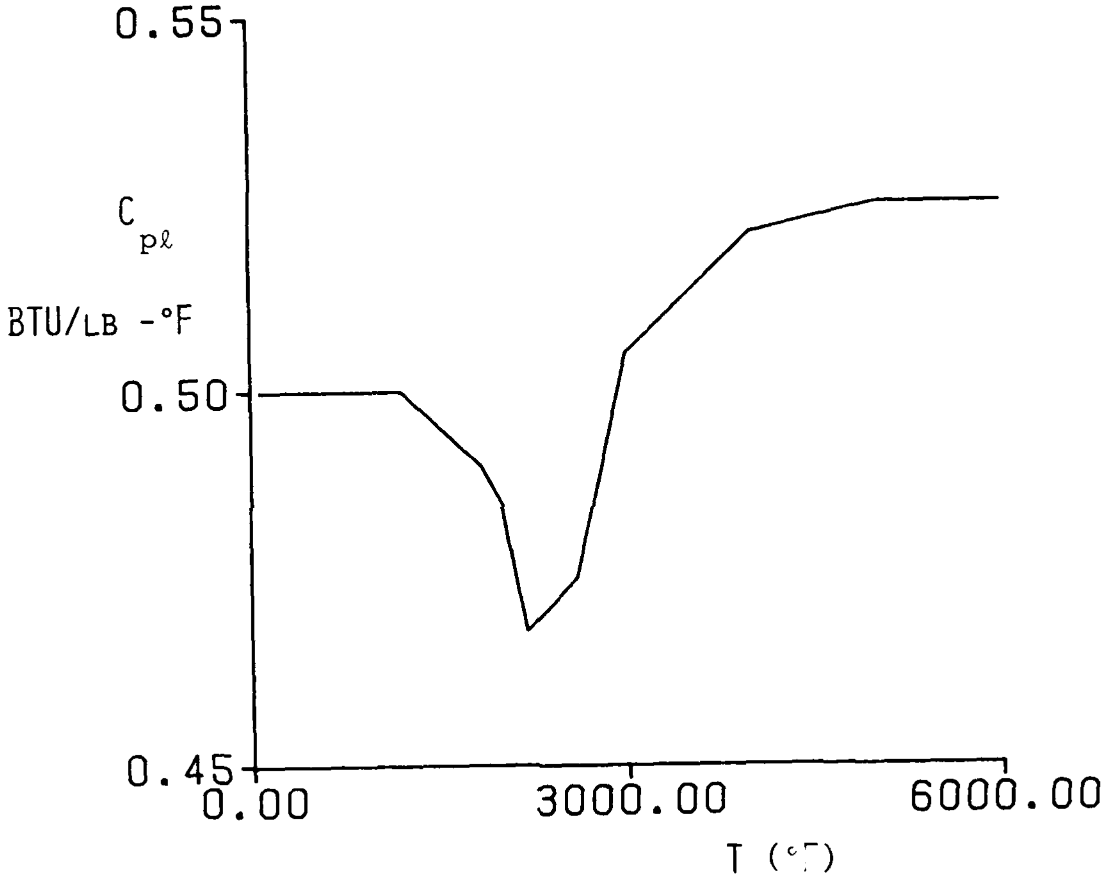


Figure 64. Liquid Pitch Specific Heat $C_{p\ell}$ Versus Temperature T.

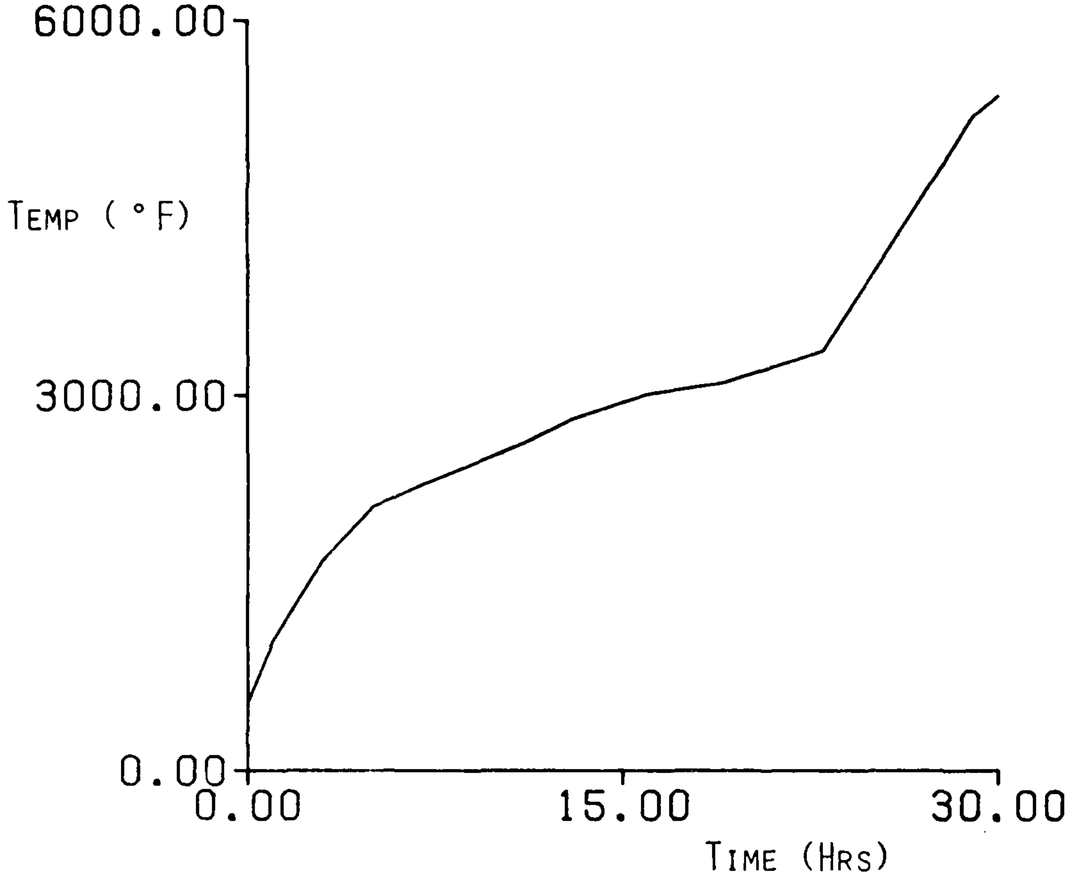


Figure 65. Graphitization Temperature Schedule.

TABLE 10

INPUT DATA FOR GRAPHITIZATION ANALYSIS OF THE BILLET SHOWN IN FIGURE 59.

```
------------------------------------------------------------------------------------------
1         10         20         30         40         50         60         70         80
?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?
------------------------------------------------------------------------------------------
1-GRAPHITIZATION EXAMPLE FOR HWP*1200 BILLET
2-    1    0    3    1    0    2    1    0
3-0.        30.       1.0       100.            1    30    0    1
4-    1    1
5-   17   13   10       0   150
6-  1  1  0.        0.       17  1  0.      0.                        1
7- 17  1  0.        0.       17 13  0.     12.                        1
8- 17 13  0.       10.        1 17  0.     10.                        1
9-  1 13  0.       10.        1  1  0.      0.                        1
10- -1
11-   1    1   17    1   13
12-   2    5   13    1   11
13-   4   17    1   17   13    1 1.0      1.0
14-   4    1   13   17   13    1 1.0      1.0
15-                           537.
16-
17-                           1.1689E-11                          180.
18-                 1.0
19-                 1.0
20-0.30      1405.4  153.      45000.
21-   1   11    0   35.2731E-070.11       0.0730
```

Cards numbering 22 to 54 are the same as Table 8, page 107.

```
55-   0   11    0   35.2731E-070.11       0.0730
```

Cards numbering 56 to 88 are the same as Table 9, page 108.

```
89-   1    12
90-0.       537.     1.      1035.4    7.    1679.4    5.    2111.4
91-7.      2091.4   11.      2615.4   13.    2813.4   16.    3111.4
92-19.     3101.4   23.      3353.4   25.    5225.4   30.    5307.4
93-END OF CASE
:----:----:----:----:----:----:----:----:----:----:----:----:----:----:----:----:
```

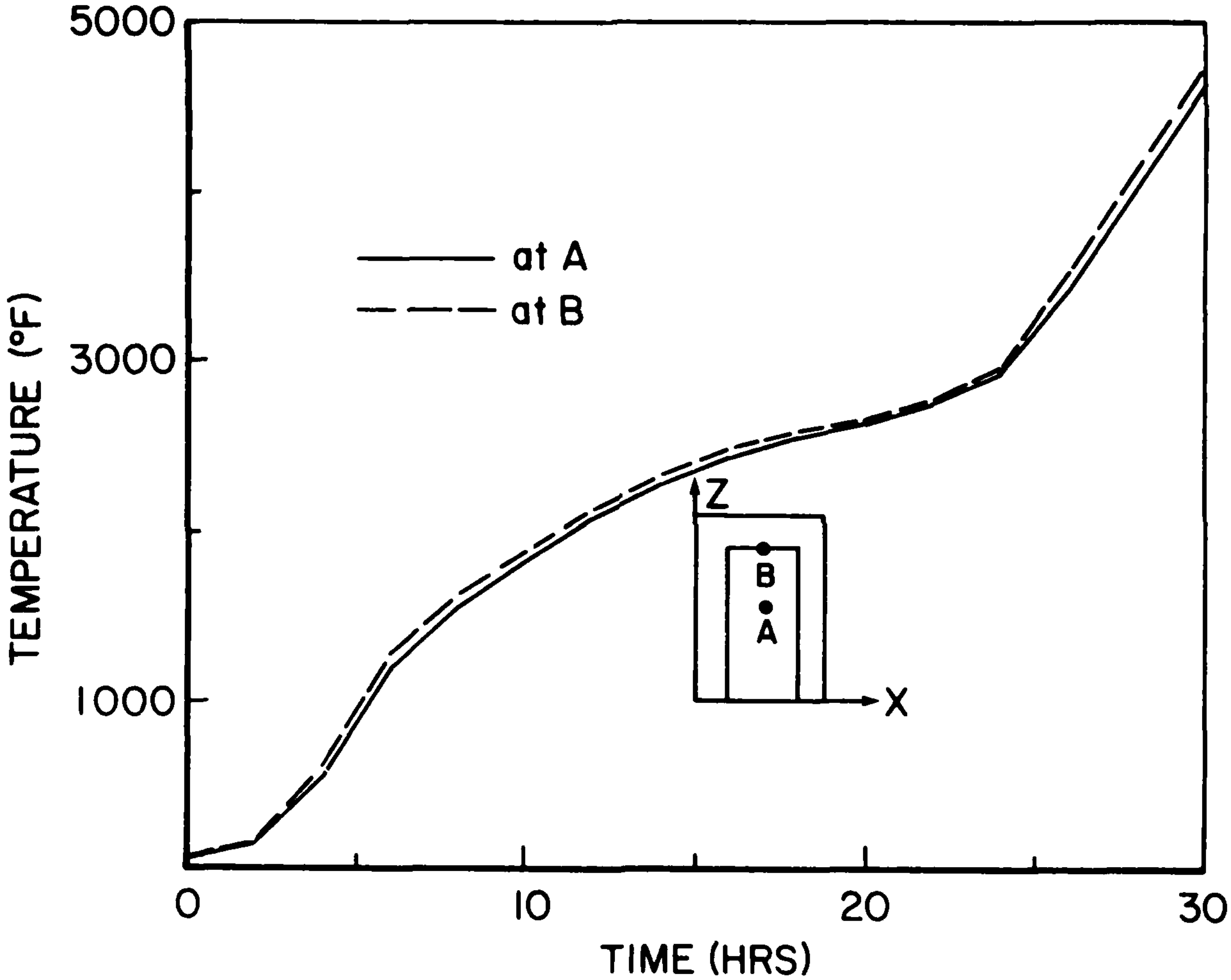


Figure 66. Temperature at Different Times at Two Locations in the Billet During Graphitization.

APPENDIX D

CLOSED FORM SOLUTIONS FOR IMPREGNATION

Governing Equations, Solutions and Results

Darcy's law for the flow of a compressible fluid through a porous media has been used for the impregnation analysis. The relevant relations [6] for this investigation are presented in this section. The governing equation of flow of a compressible fluid through porous media, in terms of pressure in the medium, will be solved for the case of uniform, isotropic and time-independent properties. The following three types of boundary conditions are treated and results compared with those obtained by using PEM code:

1. Rectangular coordinates with uniform pressure or pressure gradient at the boundaries, as shown in Figure 67.
2. Rectangular coordinates with linearly varying pressure at the outer vertical boundary and uniform pressure or pressure gradient at other boundaries as shown in Figure 68.
3. Cylindrical polar coordinates with uniform pressure or pressure gradient at the boundaries as shown in Figure 69.

Closed form solutions for all these cases of boundary value problems are obtained by Fourier transform techniques and are given on page 120 onward. Numerical results for these cases are calculated for materials with following properties:

Fluid Compressibility (C) = 1.13×10^{-5} (PSI)$^{-1}$
Fluid Viscosity (μ) = 0.24×10^{-6} lb/in^2-min.
Solid Permeability (K) = 0.75×10^{-13} in^2
Solid Porosity (ϕ) = 0.31

The problem solved for case 1 is the same as described on page 32. The numerical results obtained by using the closed form solution and the PEM code are shown in Figures 70-72. Figure 70 depicts the variation of pressure along the height of the billet (Figure 3) for x = 0 and x = 1.75". The PEM results are plotted for three values of time step length, ΔT = 1., .25 and 0.1, at the end of ten minutes impregnation. This figure shows that the accuracy of the results by PEM code improves considerably with the refinement of the time step ΔT. In the calculation of closed form solution results, the summation of series on page 120 was done for m=n=25. The magnitude of the pressure P is almost independent of m and/or n beyond 25. There exists an extremely good agreement between the closed form solution results and the PEM results with $\Delta T = 0.1$ minute. Figure 71 shows a comparison between the PEM results and the closed form solution results at T = 25 minutes. Here too, the PEM results for $\Delta T = 0.1$ minute are quite accurate. Figure 72 shows the variation of pressure, on the basis of closed form solution, at the point (0,0), of minimum pressure in the billet with time. It takes about 200 minutes before the pressure at all points of the billet reaches the value of p = 89.998.

Similar observations are made in case 2 in which a linearly varying horizontal pressure at the outer vertical boundary of the billet is considered, Figure 68. A comparison between PEM and closed form results is given in Figures 73, 74, and 75. Table 11 shows the PEM input data for impregnation analysis of a billet with a linearly varying horizontal pressure at the vertical boundary as shown in Figure 68. The billet geometry considered here is the same as that in the foregoing illustration, case (1), $P_o = 90$ and $\gamma = 45$. Figure 75 shows the variation of pressure P at (0,0) with time, calculated by the closed form solution. Thus, it takes about 200 minutes before the pressure at (0,0) reaches the value of P = 134.997, close to the applied pressure P = 135 at (2,0).

The problem solved for case 3, a billet in cylindrical polar coordinates, is shown in Figure 69. The finite element grid in the rz-plane used for the process environment model is shown in Figure 76. The PEM input data for this problem is given in Table 12. The material properties used for this case are the same as those used for the case 1. The closed form solution for this problem with relevant boundary conditions is given on page 124. This solution is expressed in terms of Bessel functions. For obtaining the roots of equation 4 page 124, a CDC mathematics library subroutine was used. During the computation of results, the series summation was done for i=m=25. As before, the results do not vary with the increase in the summation of number of terms over m or i beyond 25. Figures 77-80 show the variation of pressure P calculated by the PEM code and the closed form solution at different points of the billet. Figure 77 shows the effect of the change in the time march step ΔT. Further, it shows that the results for time step length $\Delta T = 0.1$ minute are very close to the closed form solution results. Figures 78 and 79 demonstrate the difference between the PEM results with $\Delta T = 1.0$ and .25 and the closed form solution results at $T = 20$ and 40 minutes. Figure 80 gives the change in pressure at the point of minimum pressure with respect to the time T calculated on the basis of the closed form solution. It takes about 315 minutes to reach a value of $P = 89.636$.

The governing equations for the flow of compressible fluid through a porous medium are given below:

The flux density $\nu_\xi = -\frac{K\rho}{\mu}\frac{\partial P}{\partial \xi}$ $(\xi = x, y, z)$

where

$$\rho = \rho_0 e^{C(P-P_0)}$$

ρ_0 = Fluid density at Reference pressure P_0

C = Compressibility constant $= \frac{1}{\rho}\frac{\partial \rho}{\partial P}$

K = Permeability of the material

μ = Fluid viscosity

The flow of compressible liquid through an isotropic incompressible medium in terms of pressure is governed by (Darcy's Law)

$$\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} + \frac{\partial^2 P}{\partial z^2} = \frac{\phi\mu C}{K}\frac{\partial P}{\partial T}$$

(x,y,z) - Cartesian coordinates, T = time

ϕ = porosity of the material

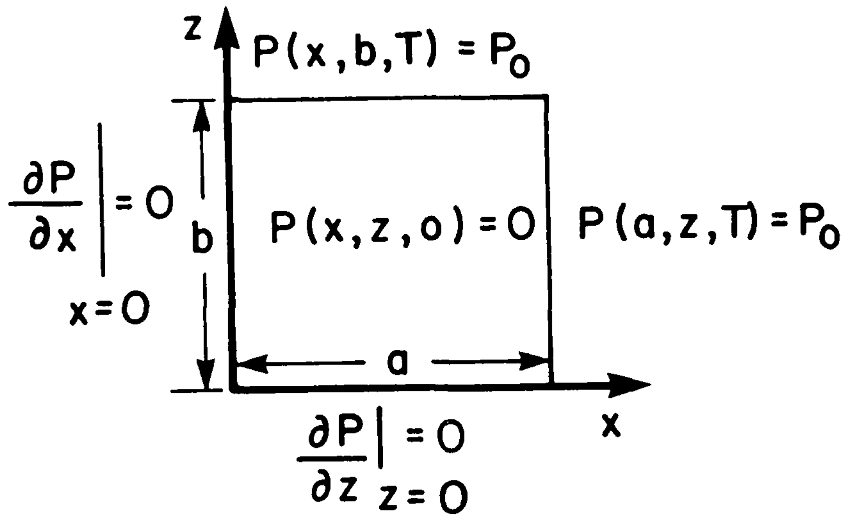


Figure 67. Coordinate Axis and Pressure Boundary Conditions for a Rectangular Billet Impregnation Analysis.

Case 1: Consider a two-dimensional case in which a quadrant of the billet has been modeled. The initial and boundary conditions are shown in Figure 67. Using Fourier transform technique the solution to this problem is:

$$P = P_0 \left[1 - \frac{4}{ab} \left\{ \sum_{n=0}^{\infty} \frac{(-1)^n}{\alpha} e^{-\alpha^2 T/k} \cos \alpha x \right\} \left\{ \sum_{m=0}^{\infty} \frac{(-1)^m}{\beta} e^{-\beta^2 T/k} \cos \beta z \right\} \right]$$

$$\alpha = \frac{(2n+1)\pi}{2a}, \quad \beta = \frac{(2m+1)\pi}{2b}, \quad k = \frac{\phi \mu C}{K}$$

Case 2: Consider a 2D case in which the pressure boundary condition at x=a is given by equation (1) as shown in Figure 68.

$$P(x,b,T) = P_0$$

$$P(a,z,T) = P_0 + \gamma\ (b-z) \qquad -(1)$$

$$\frac{\partial P}{\partial x}\Big|_{x=0} = 0$$

$$\frac{\partial P}{\partial z}\Big|_{z=0} = 0$$

$$P(x,z,0) = 0$$

The solution of this boundary value problem is:

$$P(x,z,T) = P_0+\gamma(b-z)-\frac{4}{ab}\sum_{m=o}^{\infty}\sum_{n=o}^{\infty} A_{mn}\text{Cos}\lambda_m x\ \text{Cos}\mu_n z\ e^{-(\lambda_m^2+\mu_n^2)T/k}$$

where

$$\lambda_m = \frac{2m+1}{2a}\pi,\ \mu_n = \frac{2n+1}{2b}\pi$$

$$A_{mn} = \left\{ P_0\ \frac{(-1)^n}{\mu_n} + \frac{\gamma}{\mu_n^2} \right\} \frac{(-1)^m}{\lambda_m}$$

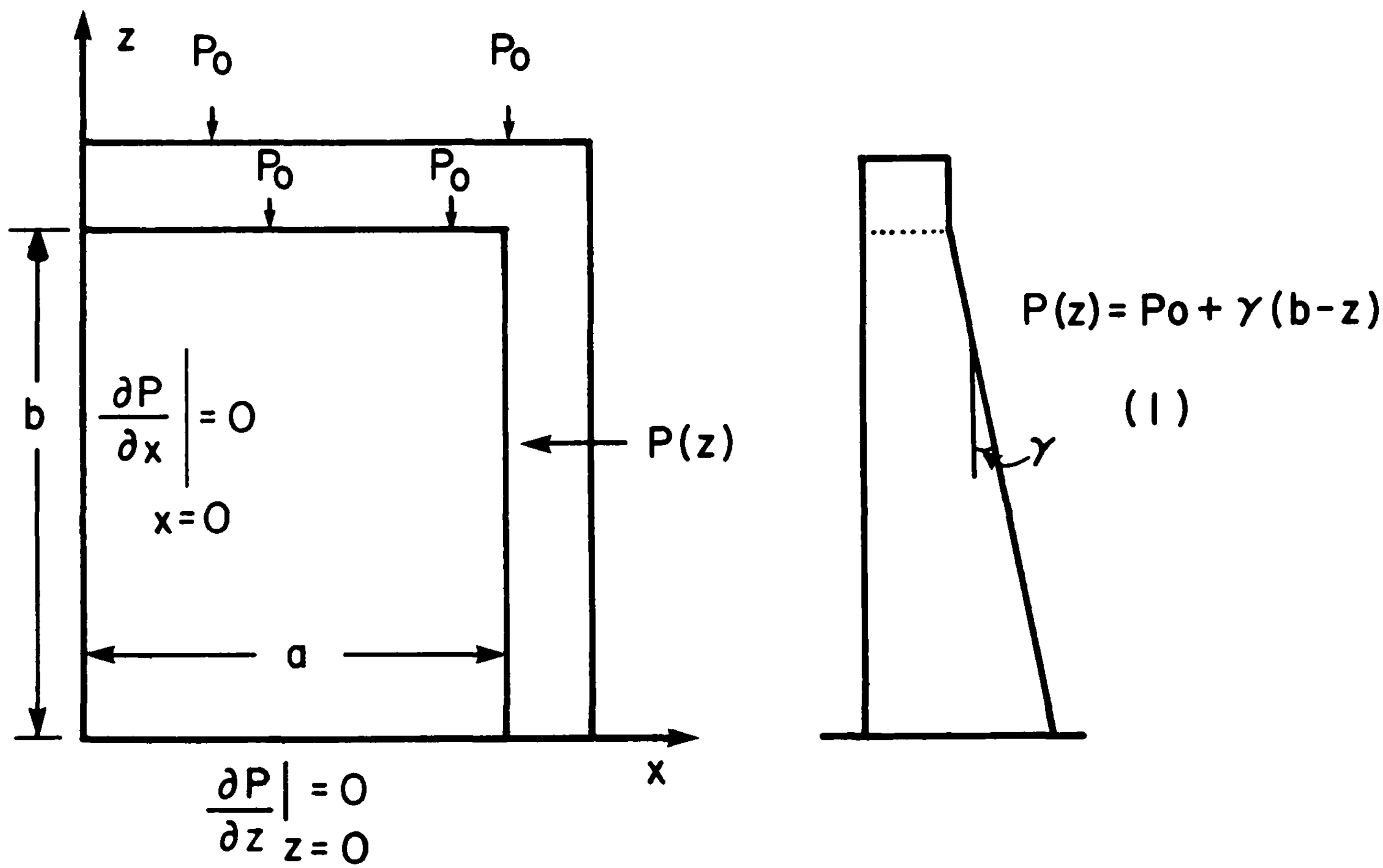


Figure 68. Boundary Conditions for Impregnation Problem with Linearly Varying Pressure at Surface x = a.

Case 3: The field equation for a cylindrical billet in Figure 72 can be written as

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial P}{\partial r}\right) + \frac{\partial^2 P}{\partial z^2} = k\frac{\partial P}{\partial T} \qquad (1)$$

The solution for the boundary value problem given in Figure 72 is:

$$P(r,z,t) = q_0\left[1- \sum_{i=1}^{\infty}\sum_{m=0}^{\infty}\frac{(-1)^m 4b}{\ell\mu_m\lambda_i}\frac{R_1(b\lambda_i)R_0(\lambda_i r)\cos\mu_m z}{\{b^2R_0'^2(\lambda_i b)-a^2R_0^2(\lambda_i a)\}}e^{-(\lambda_2^2+\mu_m^2)T/k}\right]$$

$$\mu_m = \frac{2m+1}{2\ell}\pi \qquad (2)$$

where

$$R_n(\lambda_i r) = J_n(\lambda_i r) - \frac{J_0(\lambda_i b)}{Y_0(\lambda_i b)}Y_n(\lambda_i r) \qquad n=0,1 \qquad (3)$$

A prime means the differentiation with respect to the argument and λ_i are real roots of:

$$J_0(\lambda_i b)Y_0'(\lambda_i a) - J_0'(\lambda_i a)Y_0(\lambda_i b) = 0. \qquad (4)$$

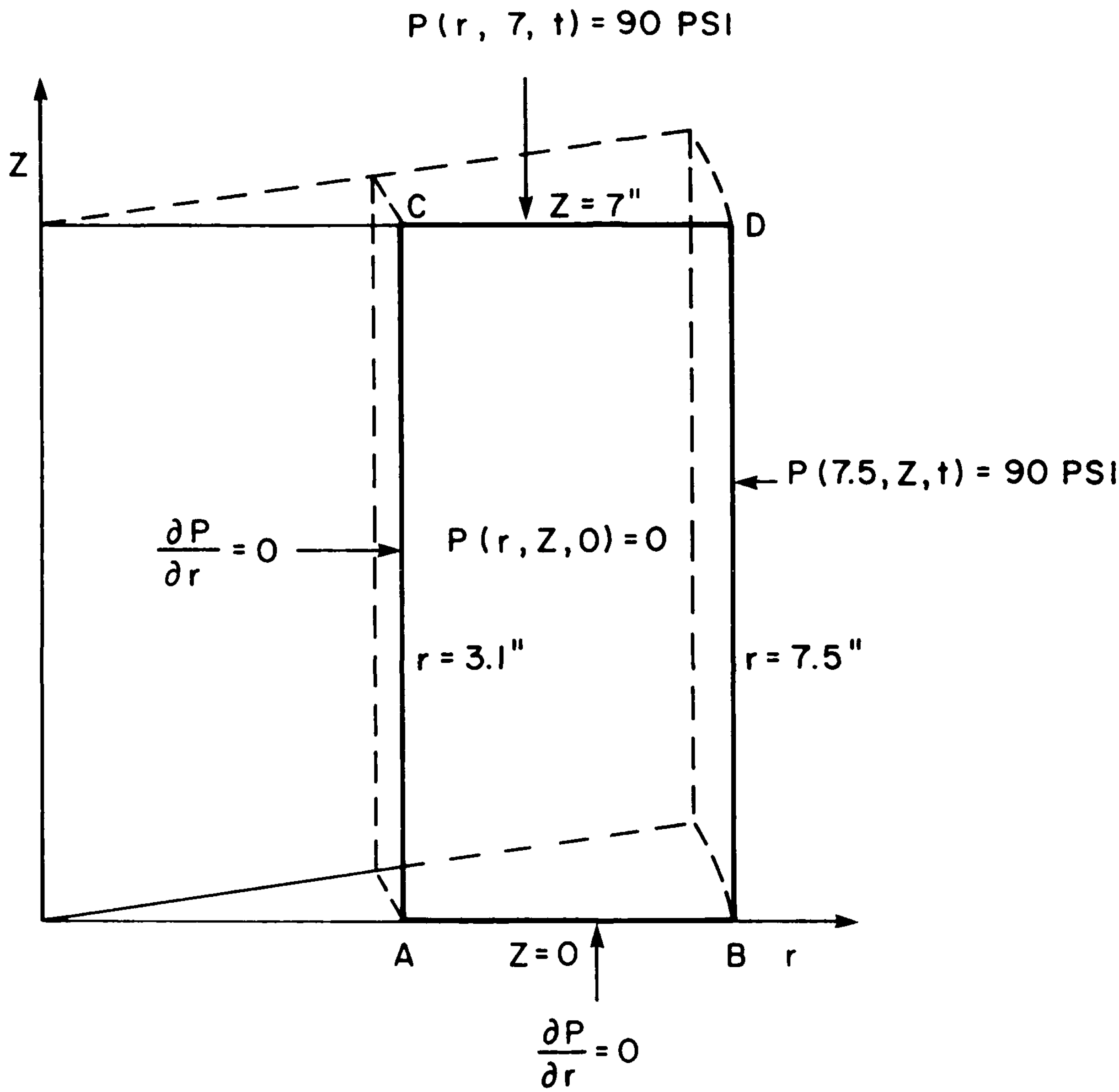


Figure 69. Cylindrical Polar Coordinates - Billet Plane Considered for the Impregnation Modeling is Shown to be Surrounded by ABCD.

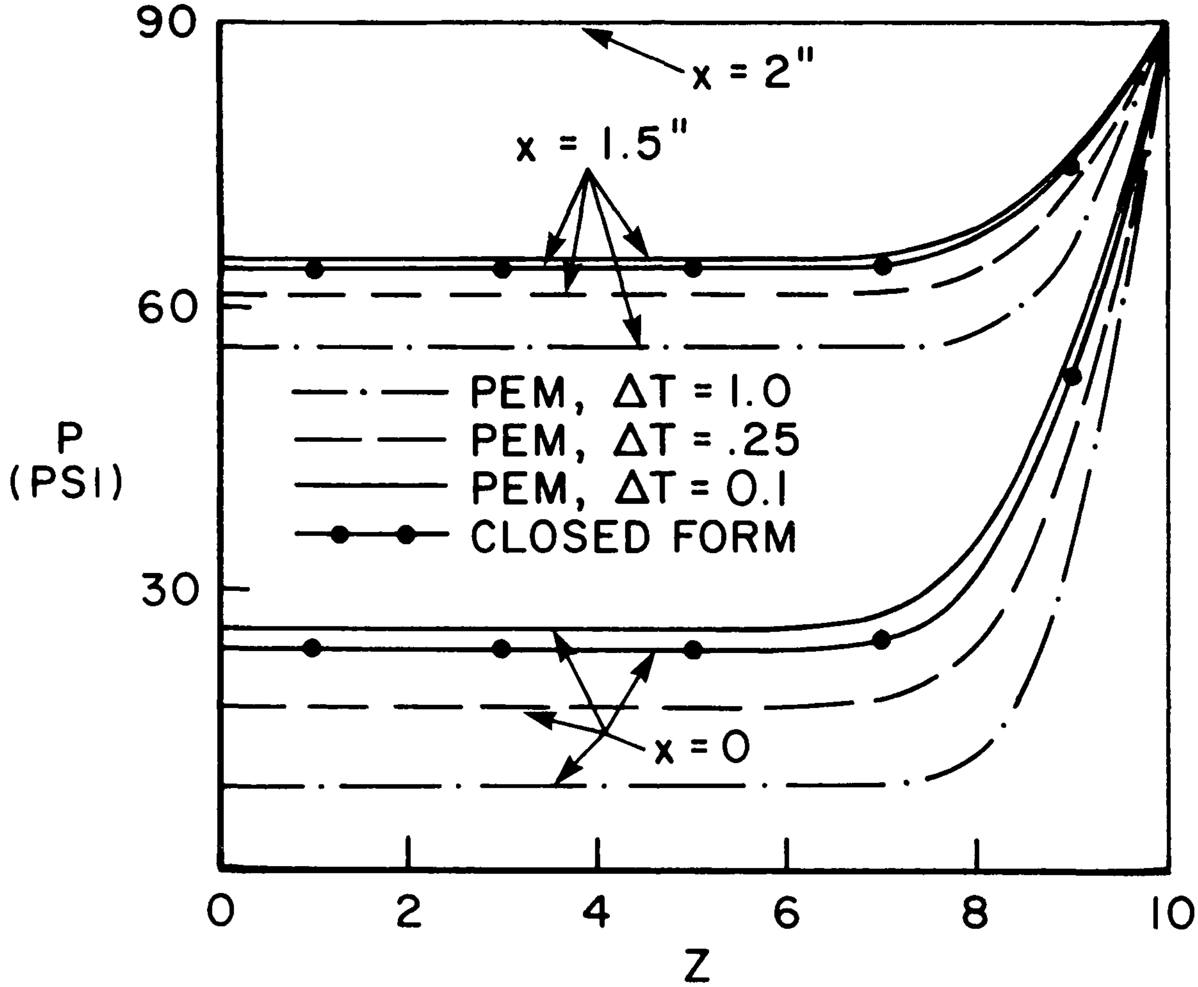


Figure 70. Comparison Between PEM and Closed Form Solution Results for Impregnation after Ten Minutes, for Case 1.

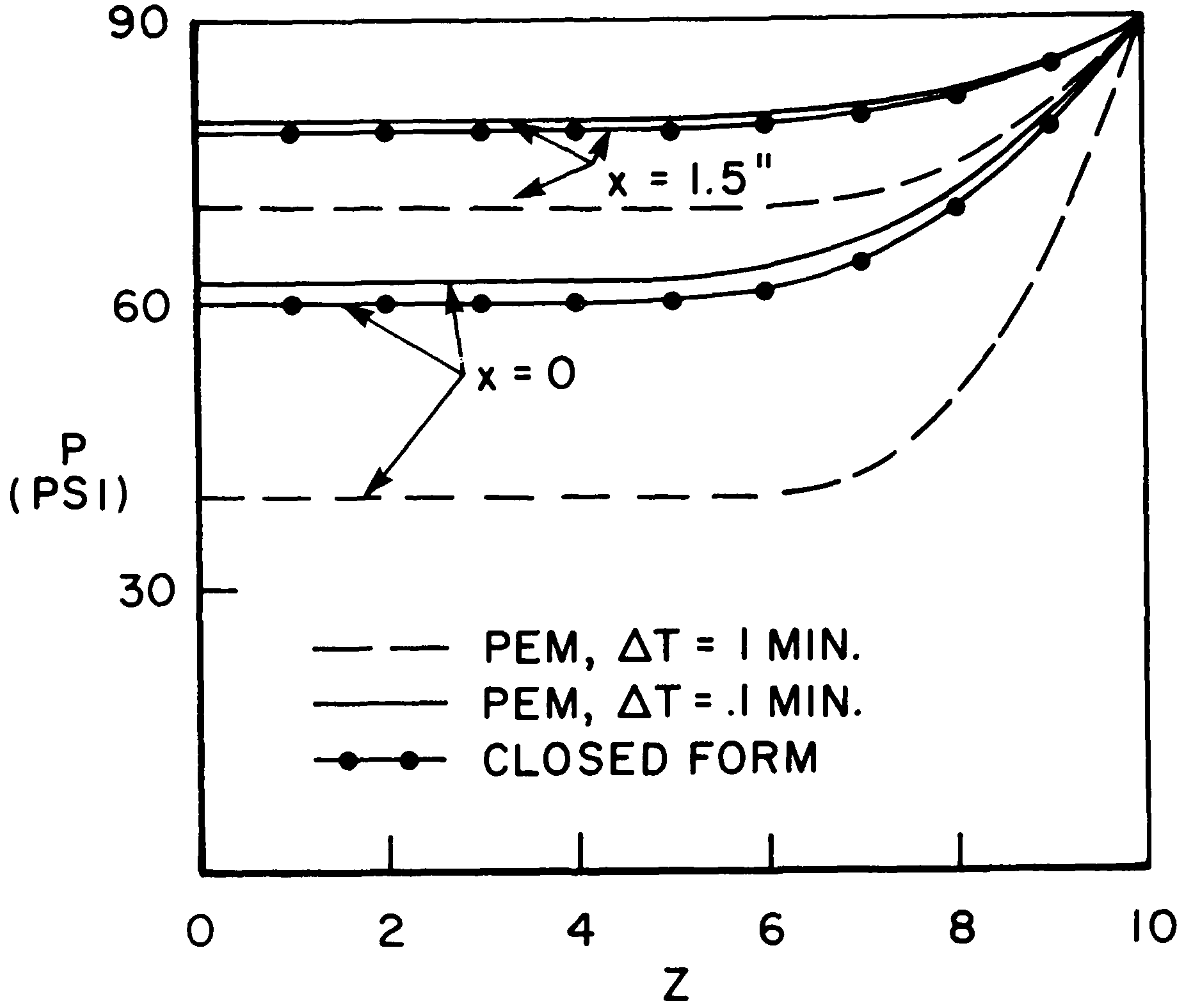


Figure 71. Comparison Between PEM and Closed Form Results for Impregnation after 25 Minutes, for Case 1.

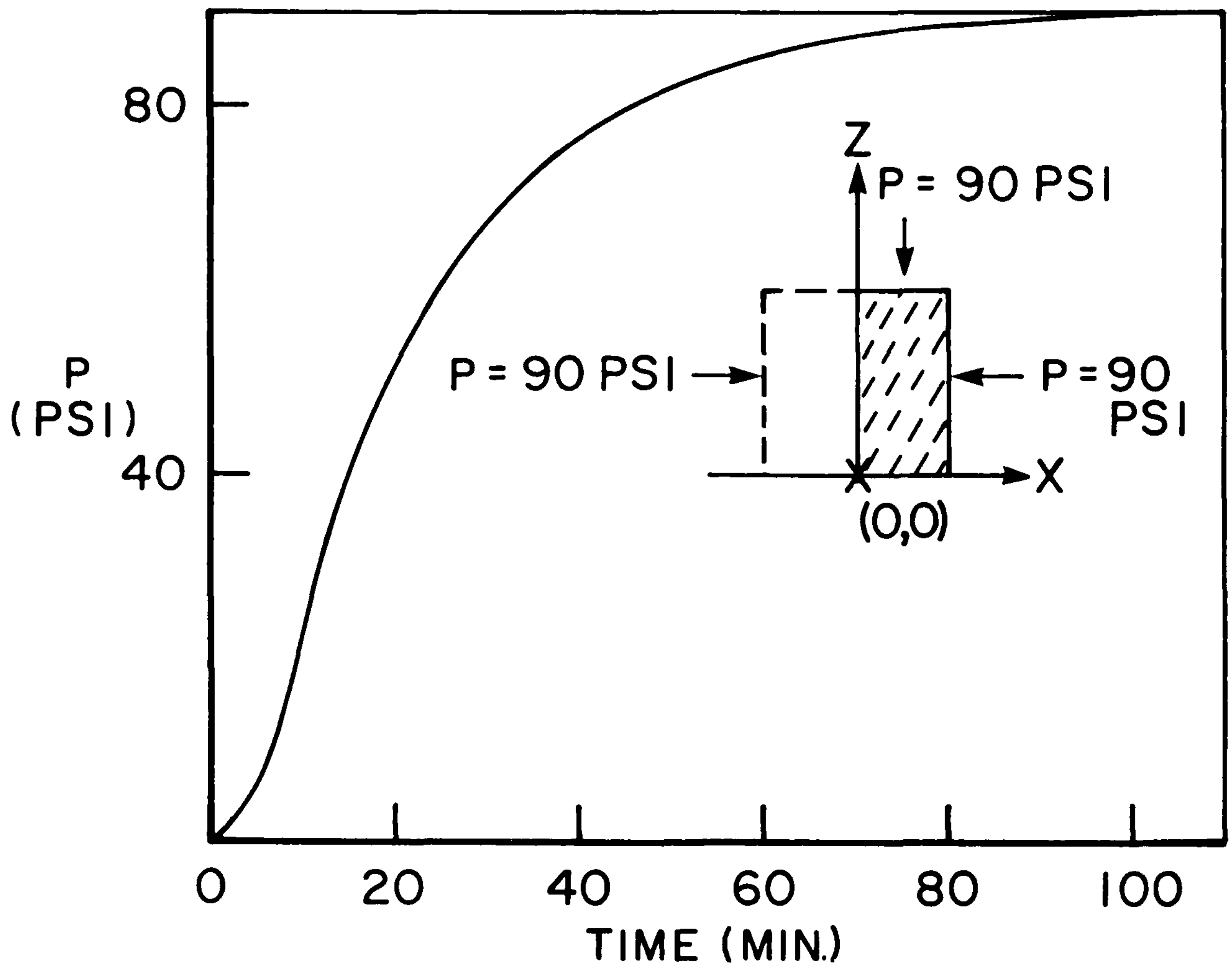


Figure 72. Pressure at the Point (0., 0.) in the Billet Versus Time During Impregnation, in Cartesian Coordinates, for Case 1.

TABLE 11

PEM INPUT DATA FOR IMPREGNATION ANALYSIS OF A RECTANGULAR BILLET
WITH VARIABLE HORIZONTAL PRESSURE

I M A G E S   O F   D A T A   C A R D S   F O R   N C A S E   = 1

```
     --------------------------------------------------------------------------------
     1        10        20        30        40        50        60        70        80
     ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?
     --------------------------------------------------------------------------------
 1-    AMVION BILLET                                                                   -
 2-       1    0    0    2    0    0    2    0    1                                   -
 3-0.          40.      0.10       400.         1   400    0    1                      -
 4-       1    2                                                                       -
 5-       5   11   10        1  150                                                    -
 6-   1  1  0.         0.    5  1 2.      1.                               1           -
 7-   5  1  2.    0.         5 11 2.     10.                               1           -
 8-   5 11  2.    10.        1 11 0.     10.                               1           -
 9-   1  1  0.    0.         1 11 0.     10.                               1           -
10- -1                                                                                 -
11-       1    1    5    1   11                                                        -
12-       0    5    1    5   11    0 135.     90.0                                     -
13-       0    1   11    5   11    0 90.0     90.0                                     -
14-                                                                                    -
15-                                                                                    -
16-                                                                                    -
17-                                                                                    -
18-                                                                                    -
19-                                                                                    -
20-       1    1    1    3 5.2731E-7 0.31                                              -
21-                                                  0.046586                          -
22-                         2.4155E-7         7.5000E-147.5000E-14                     -
23-END OF CASE                                                                         -
     :----:----:----:----:----:----:----:----:----:----:----:----:----:----:----:----:
```

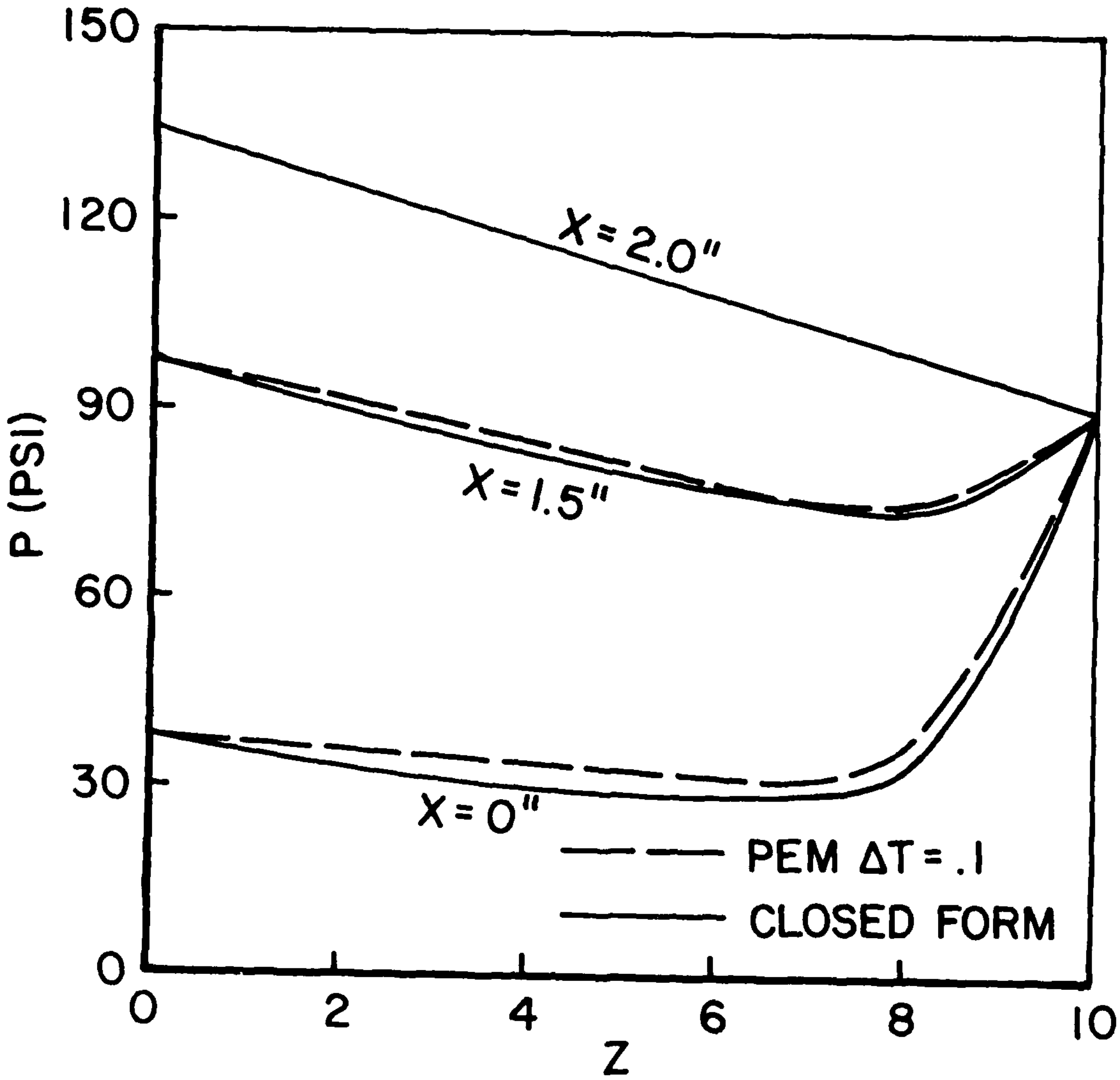


Figure 73. Comparison Between PEM and Closed Form Solution Results for Impregnation after Ten Minutes.

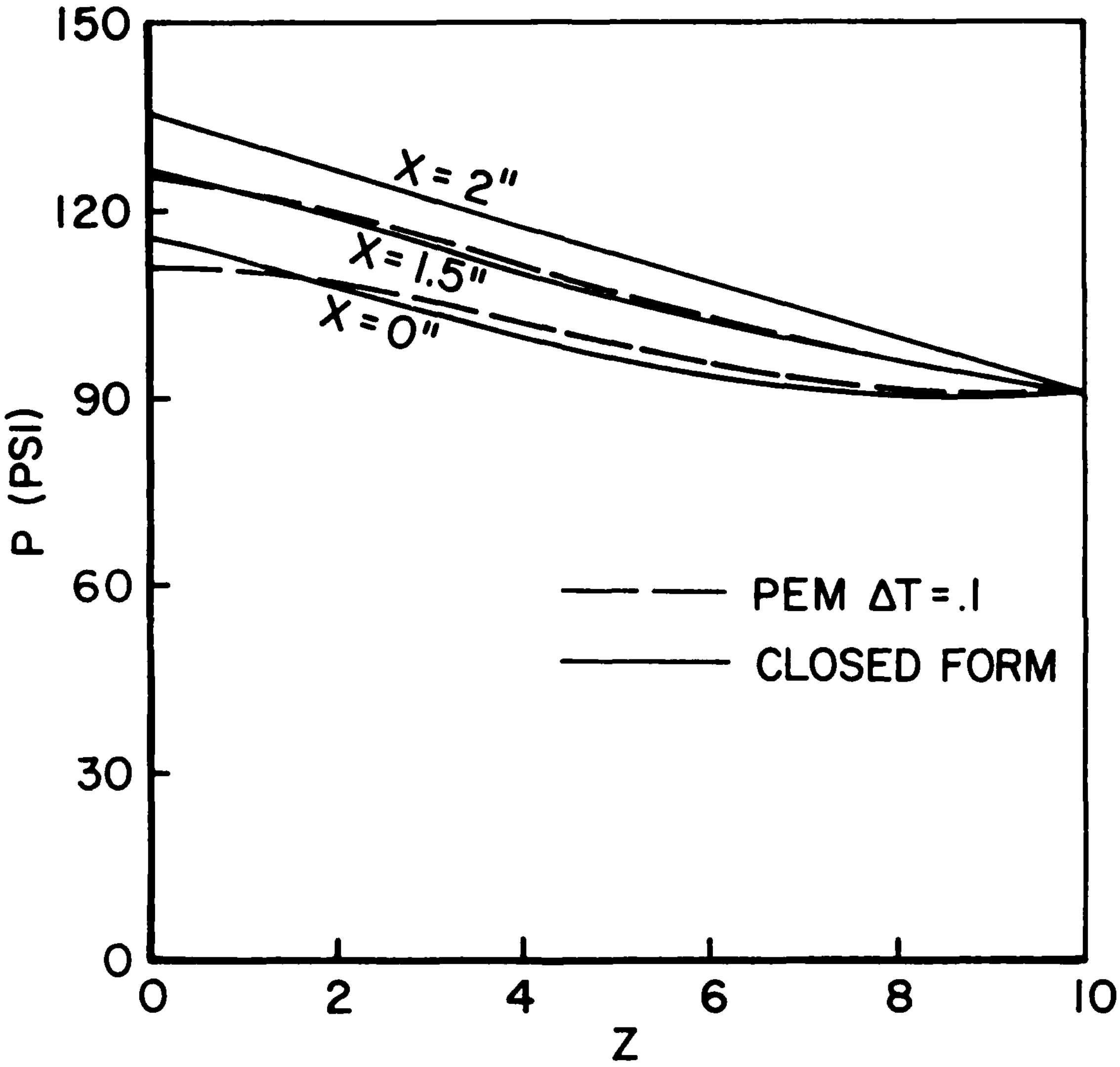


Figure 74. Comparison Between PEM and Closed Form Solution Results for Impregnation after Forty Minutes.

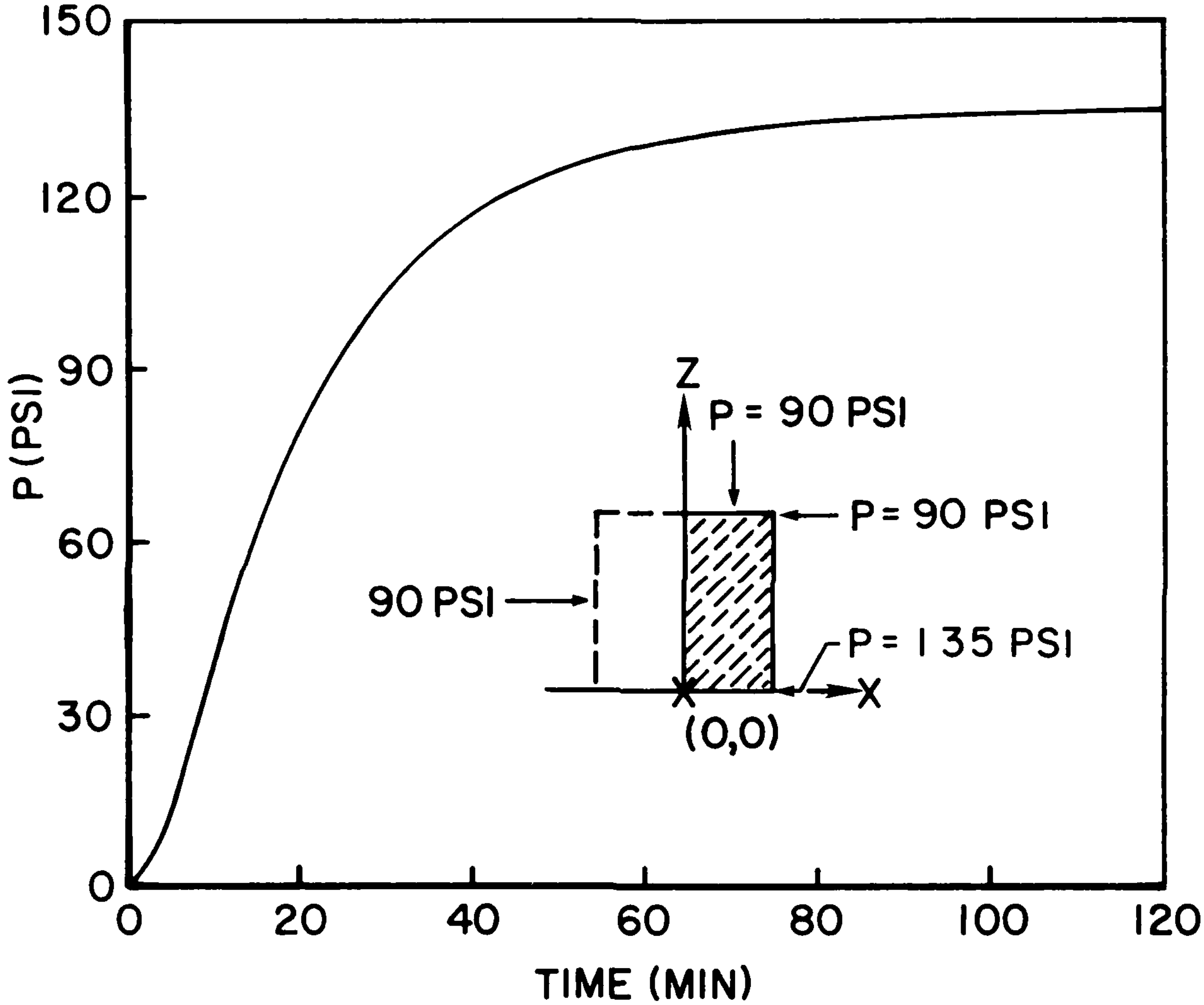


Figure 75. Pressure at the Point (0,0) in the Billet Versus Time During Impregnation, Cartesan Coordinates.

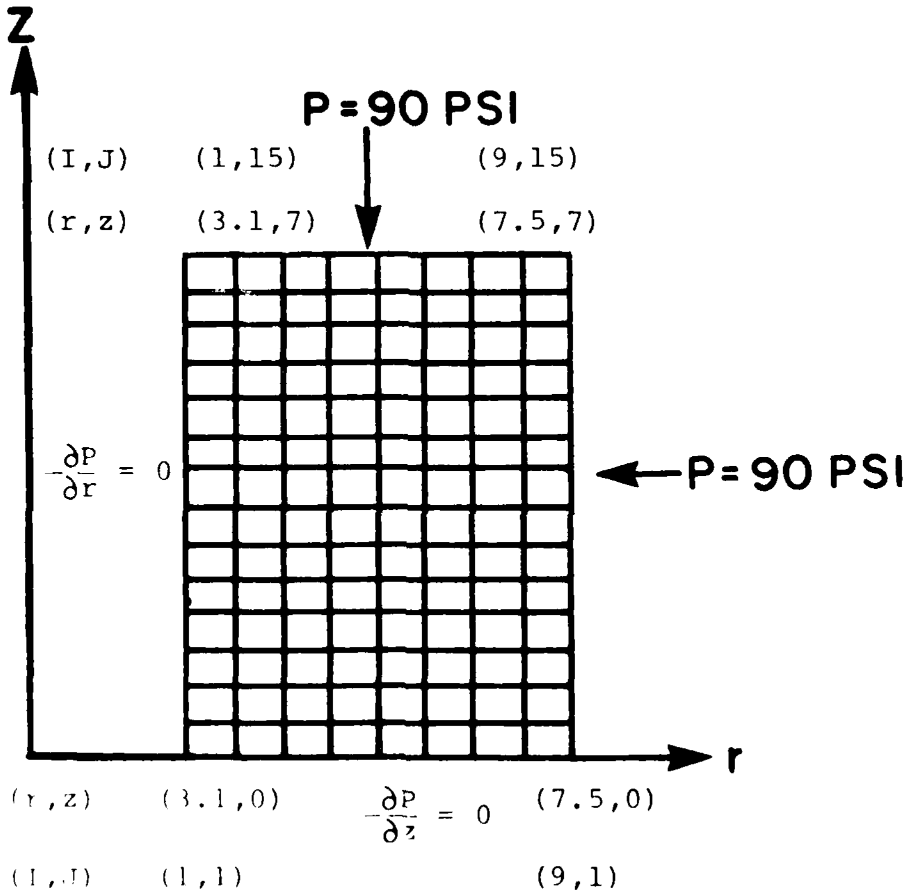


Figure 76. Finite Element Grid for a Cylindrical Billet.

TABLE 12

PEM INPUT DATA FOR IMPREGNATION ANALYSIS OF A
CYLINDRICAL BILLET GIVEN IN FIGURE 73

```
     ---------------------------------------------------------------------------------
     1        10        20        30        40        50        60        70        80
     ?   ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?    ?
     ---------------------------------------------------------------------------------
  1-  CYLINDRICAL BILLET
  2-         1         0    0    0    2    0    1
  3- .       10.       1.6       100.           1  100    0    1
  4-    1    2
  5-    9   15   15         1  150
  6-  1  1 3.1   0.         9  1 7.5      0.                              1
  7-  9  1 7.5   0.         5 15 7.5      7.                              1
  8-  9 15 7.5   7.         1 15 3.1      7.                              1
  9-  1  1 3.1   0.         1 15 3.1      7.                              1
 10- -1
 11-    1    1    5    1   15
 12-    2    9    1    9   15     0 90.      90.
 13-    2    9   15    1   15     0 90.      90.
 14-
 15-
 16-
 17-
 18-
 19-
 20-    1    1    1    3 5.2731E-7 0.31
 21- 0.                                               .046586
 22-                     2.4155E-7             7.5E-14   7.5E-14
 23- END OF CASE
     :----:----:----:----:----:----:----:----:----:----:----:----:----:----:----:----:
```

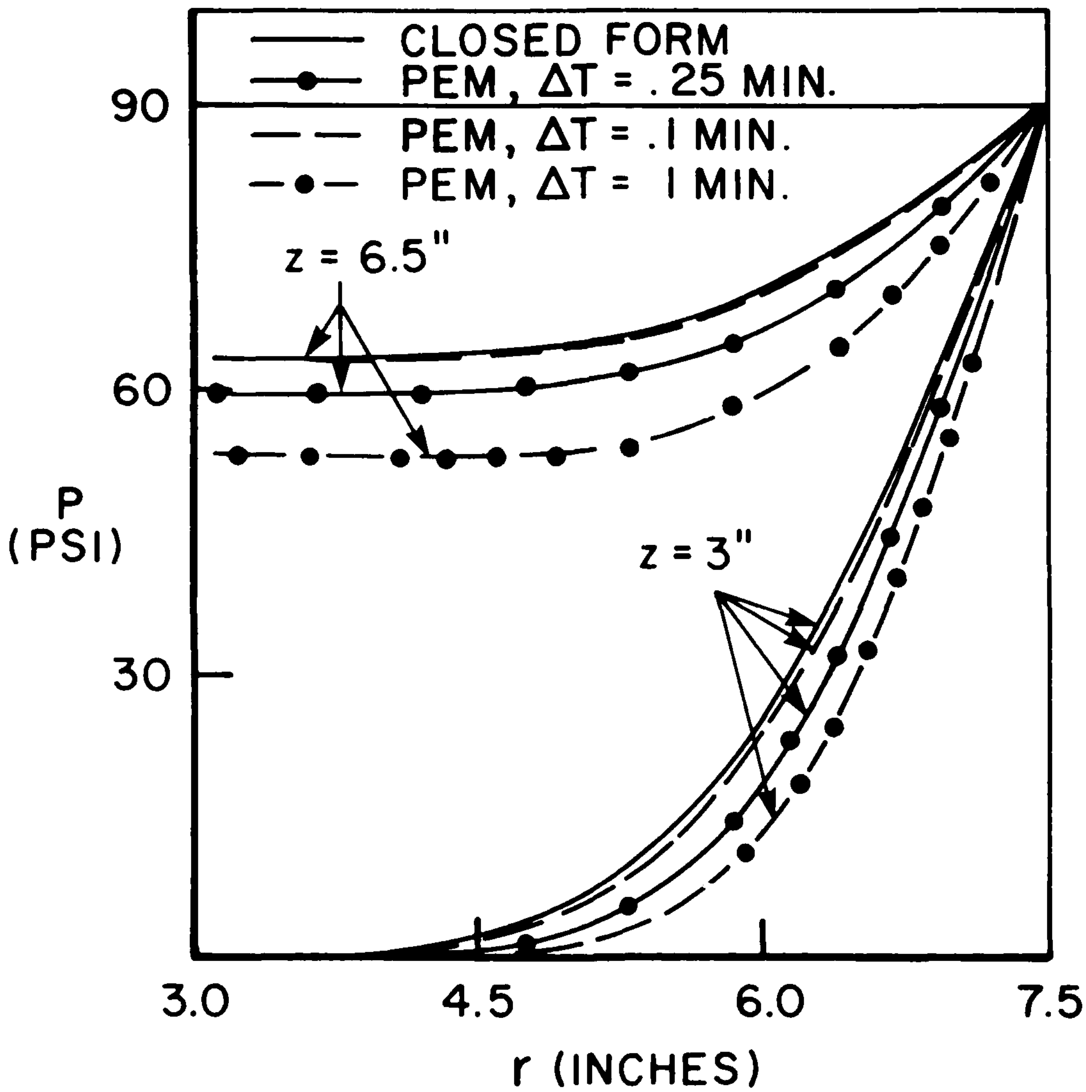


Figure 77. Comparison of Predicted Pressure Profiles Between the Closed Form and PEM Results after Ten Minutes of Impregnation.

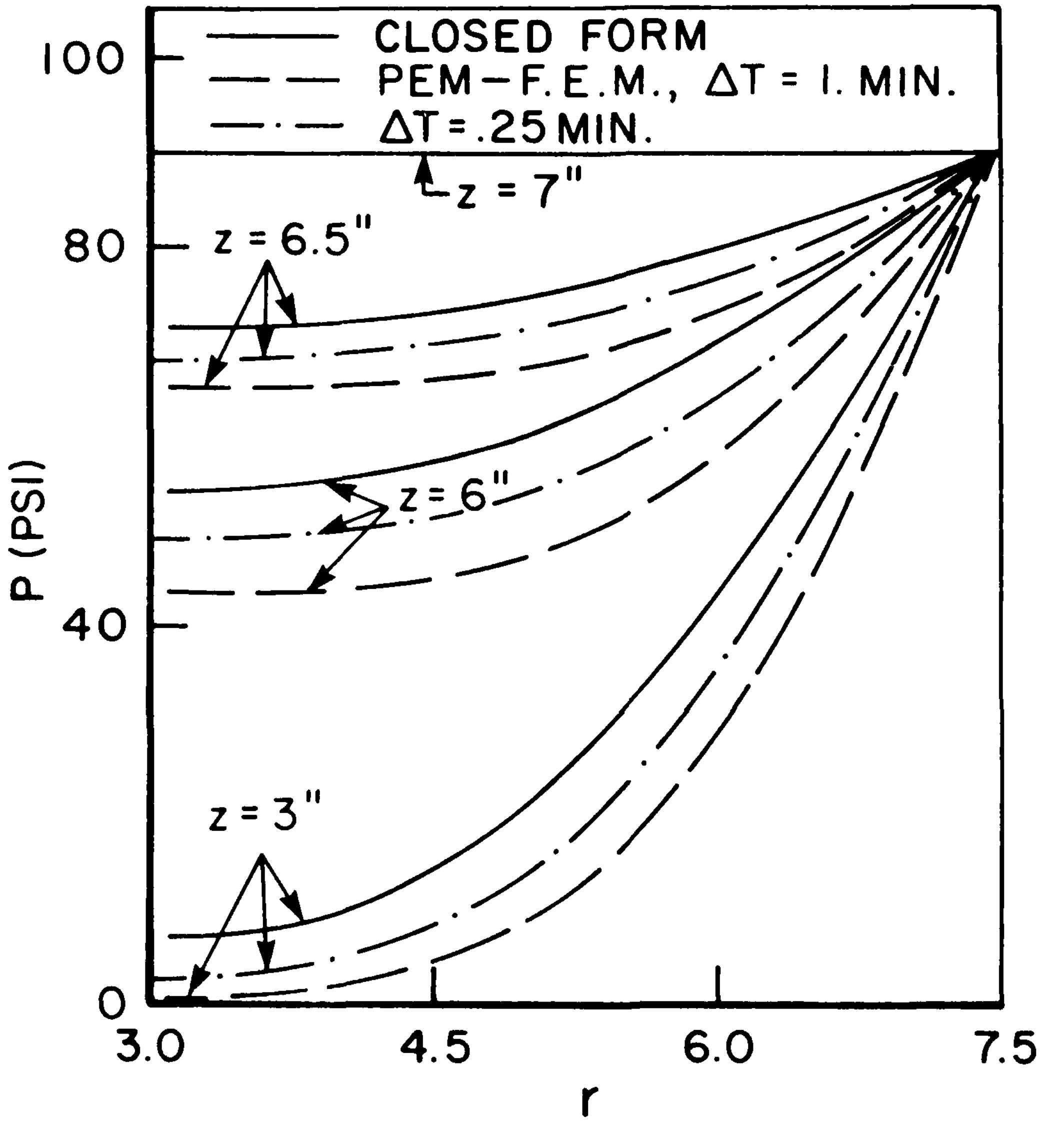


Figure 78. Comparison of Pressure Results, for Impregnation Studies in Cylindrical Polar Coordinates, Between the Closed Form and PEM Calculations after Twenty Minutes.

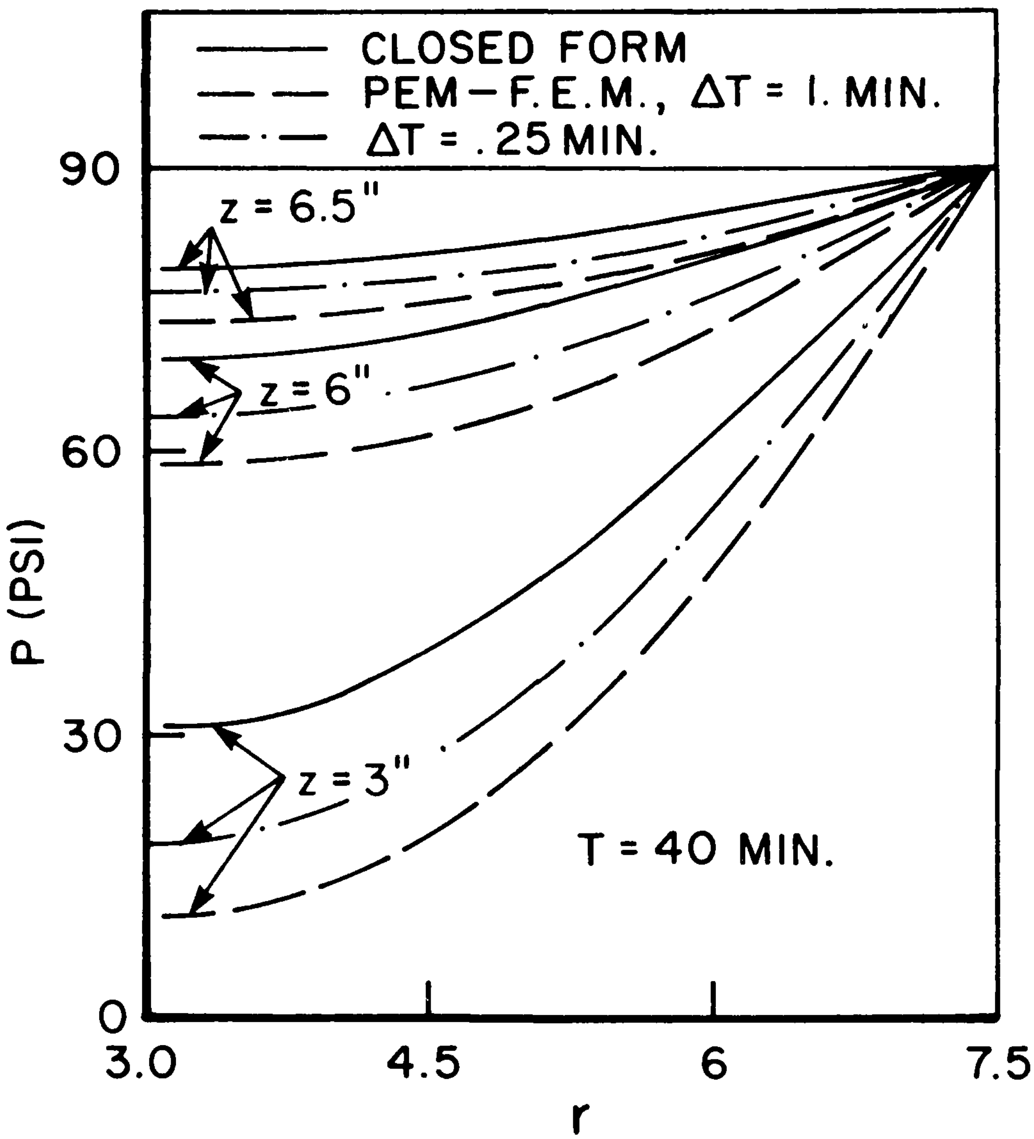


Figure 79. Comparison of Results, for Impregnation Studies in Cylindrical Polar Coordinates, Between the Closed Form and PEM Calculations, T = 40 min.

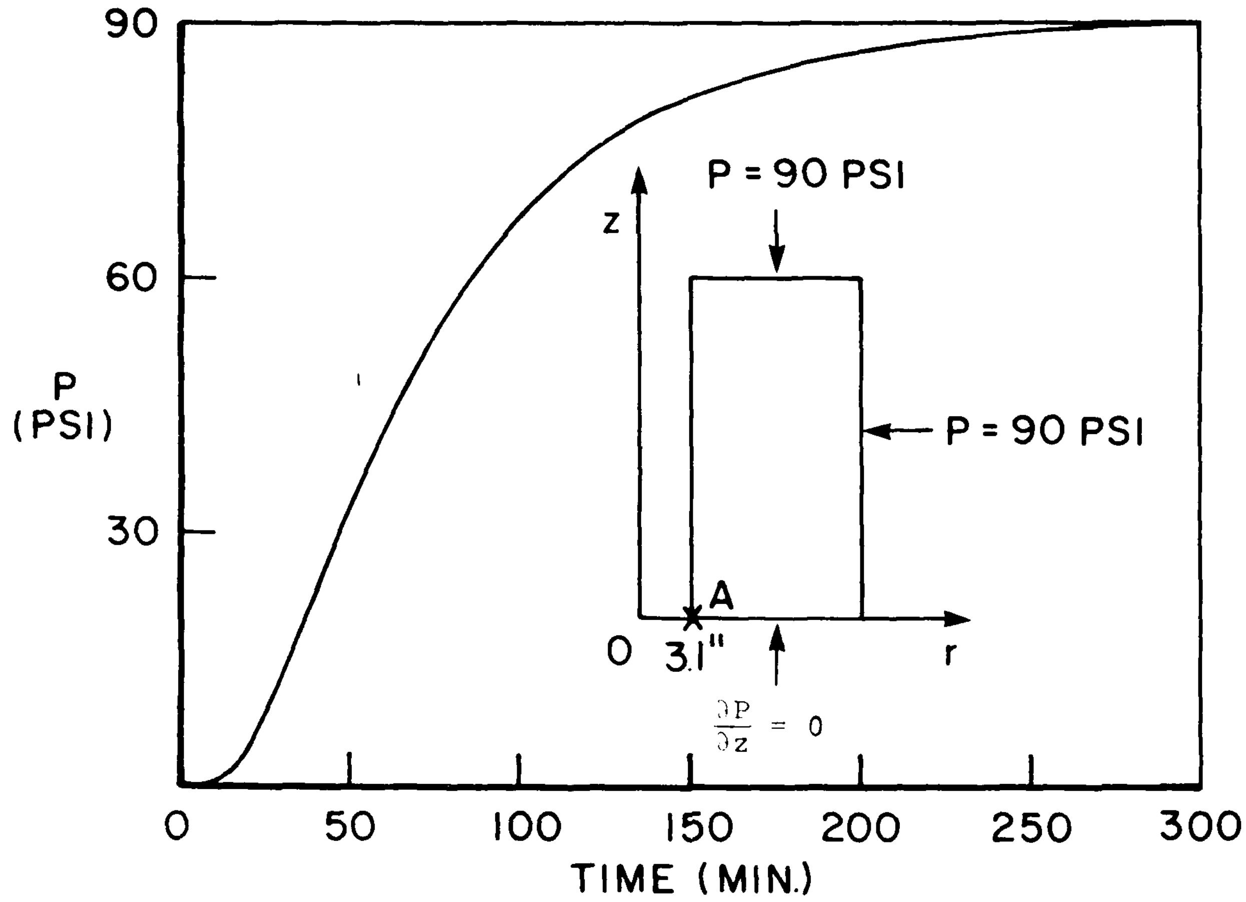


Figure 80. Pressure Variation at A (3.1, 0) in the Billet Versus Time During Impregnation in Cylindrical Coordinates.

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